Electronic Properties of the Material Computational Approach
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Module No # 07
Lecture No # 33
Semiclassical Electron Dynamics: Concept of Electron and Hole Orbit

Hello friends I already have discussed about electrons and holes in this lecture I am going to introduce another important concept of electron and whole life Fermi surface and electron and whole life body. The concept of electron and whole orbit is going to explain the anomalous whole coefficient observed in divalent, trivalent and eternal metals.

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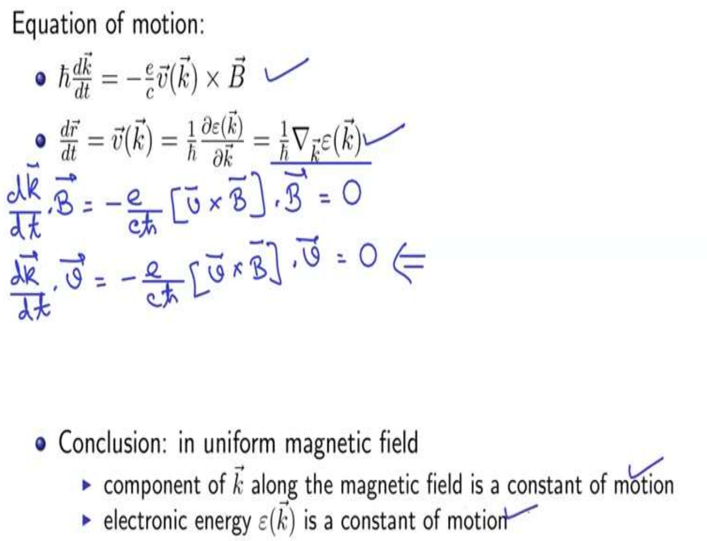

If we just have an external magnetic field then equations of motion are given by this and this. Let us calculate d k d t dot B which is equal to 0. Thus, component of K parallel to B does not change with time or in other words component of K along the magnetic field is a constant of motion. Next, we calculate d k d t dot v where v is the velocity this is equal to which is equal to 0.

$$\frac{d\vec{k}}{dt}\vec{B} = -\frac{e}{c\hbar}[\vec{v} \times \vec{B}].\vec{B} = 0$$

$$\frac{d\vec{k}}{dt}\vec{v} = -\frac{e}{c\hbar}[\vec{v} \times \vec{B}].\vec{v} = 0$$

Since v is gradient of energy this equation implies that energy is also a constant of motion. In conclusion in a uniform magnetic field component of K along the magnetic field is a constant of motion and electronic energy is a constant of motion.

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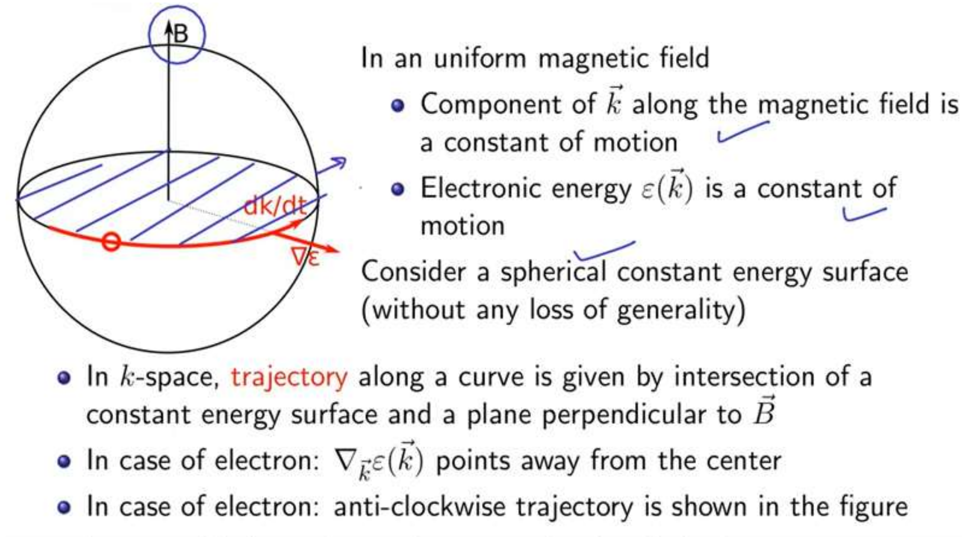

Let us consider the free electron like constant energy surface spherical in shape and understand the consequences of 2 constants of motion considering a uniform external magnetic field. However, what we are going to discuss will remain valid even if the constant energy surface is not spherical magnetic field is in this direction. Since component of K along the magnetic field does not change with type the electron orbit must be confined to a plane perpendicular to the external magnetic field that is this plane.

More over since energy is also a constant of motion the electron orbit has to stay on the constant energy surface in this case a spherical surface.

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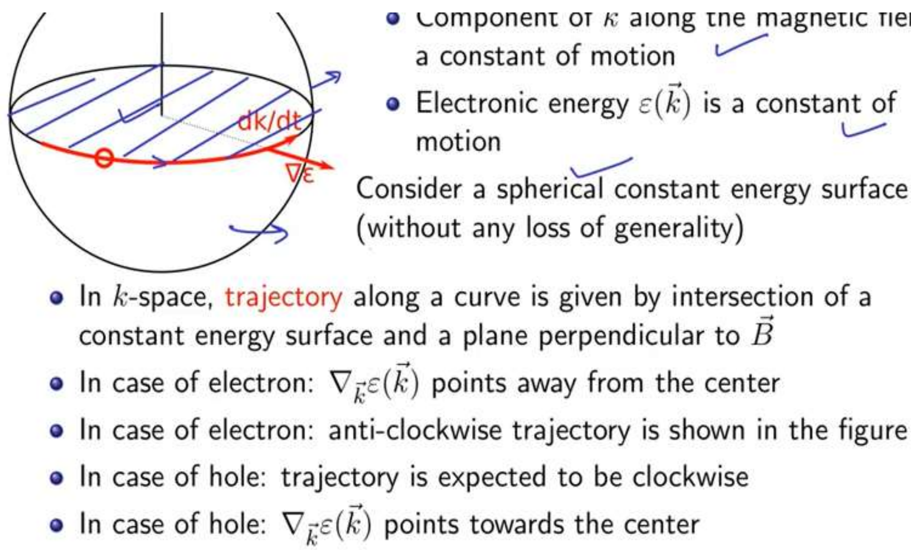

Thus in k space trajectory along a curve is given by the intersection of a constant energy surface which is spherical in this case and a plane perpendicular to B which is marked by blue lines in this diagram. The trajectory of electron is along the red curve in case of electron gradient of energy points away from the centre and the trajectory is anti-clockwise. This is known as electron like orbit a hole is positively charged and its orbit is clockwise in a magnetic field in case of a whole orbit gradient of energy points towards the center.

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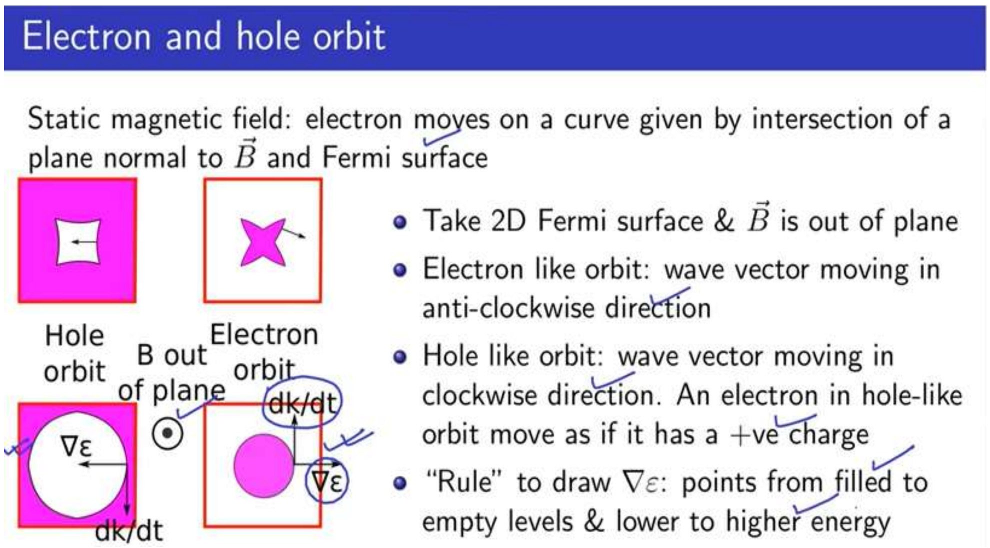

We know that in a static magnetic field electrons move on a curve determined by the intersection of a constant energy surface and a plane perpendicular to the constant energy surface it makes sense to take the constant energy surface to be the Fermi surface. Let us take a 2D Fermi surface and consider the magnetic field to be out of the plane. In these figures the shaded regions are occupied and the concerned regions are unoccupied states the closed orbits in this figure.

And in this figure are traverse in opposite directions since particles having opposite charge orbit in a magnetic field in opposite sense, we call this orbit as electron lag and this orbit as whole like. In electrolyte orbit wave vector change in a counter clockwise direction in; whole like orbit wave vector change in a clockwise direction. An electron in whole life orbit moves as if it has a positive charge note that d k d t is perpendicular to the gradient of energy.

So if we draw the gradient first, we can easily find out the orbit in k space is there any rule to draw the gradient of energy you have to keep in mind that the gradient points from field to empty levels and lower to higher energy.

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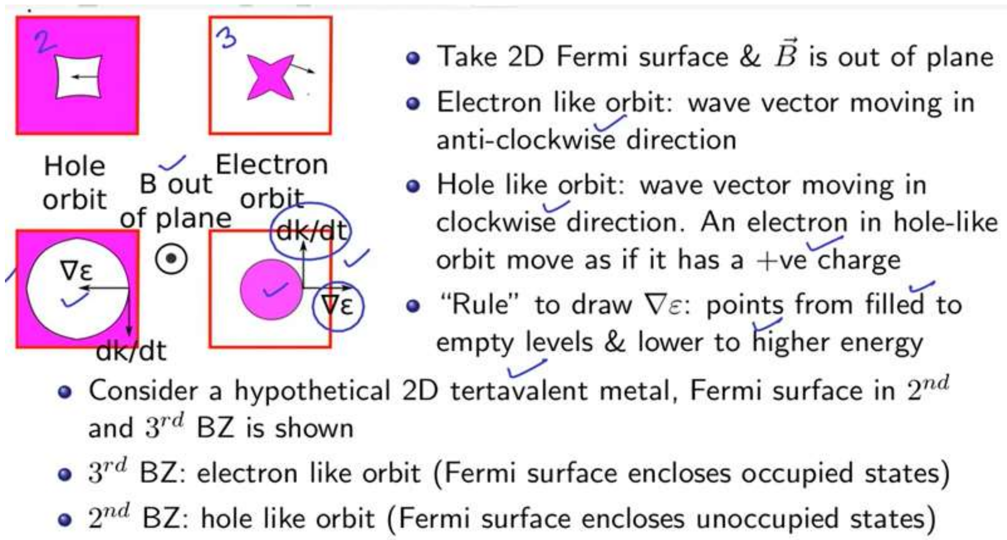

Note that, if the Fermi surface encloses field states it is an electron like Fermi surface and the orbit is electron like orbit. On the other hand if the Fermi surface encloses unoccupied states, it is a whole like Fermi surface and the orbit is whole like orbit whatever we have discussed applies to Fermi surface of any shape. For example, take a hypothetical 2d tetravalent metal, I have already shown how to draw the free electron Fermi surface for a 2d tetravalent matter.

This is how the Fermi surface looks like in the second Brillouin zone and this is how it looks like in the third Brillouin zone. The first Brillouin zone is completely full and not shown here in secondary Brillouin zone. We have a whole like Fermi surface this is the gradient and dkdt points in this direction. In third Brillouin zone we have an electron light Fermi surface this is the gradient and decadity points in this direction.

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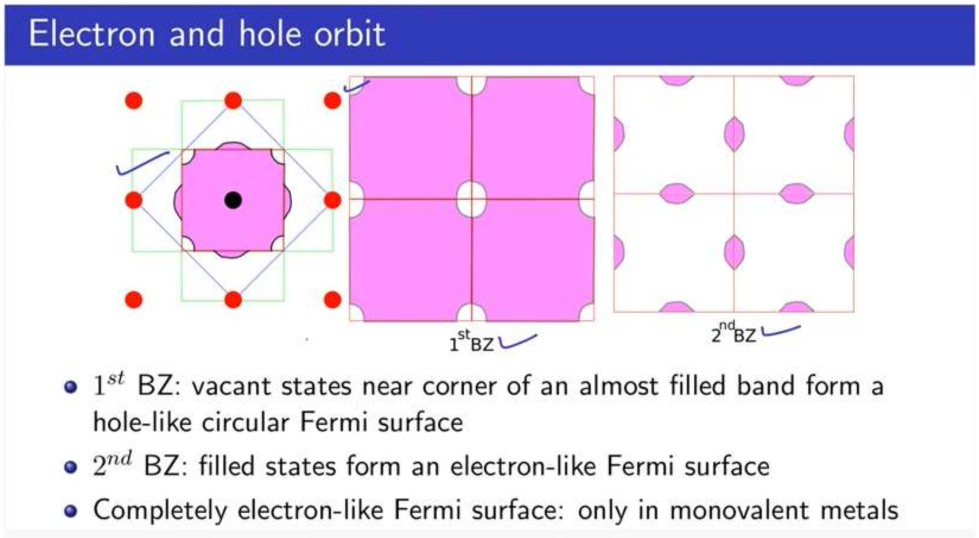

Let us consider a divalent metal. We already know how to draw the Fermi surface of a divalent metal this is how it looks like in extended zone scheme part of the Fermi surface lies in the first Brillouin zone and rest of it in the second Brillouin zone. So, if we repeat periodically in reciprocal space this is how it looks like in the first Brillouin zone. And this is how it looks like in the second Brillouin zone clearly there are vacant sites near the corner of an almost feet bent.

As a result, we get a whole like Fermi surface in the first Brillouin zone so note that Fermi surface is enclosing empty states in this case. On the other hand there are some occupied states in the second Brillouin zone, as a result, we get an electron like Fermi surface in second Brillouin zone note that Fermi surface is enclosing field states in this case.

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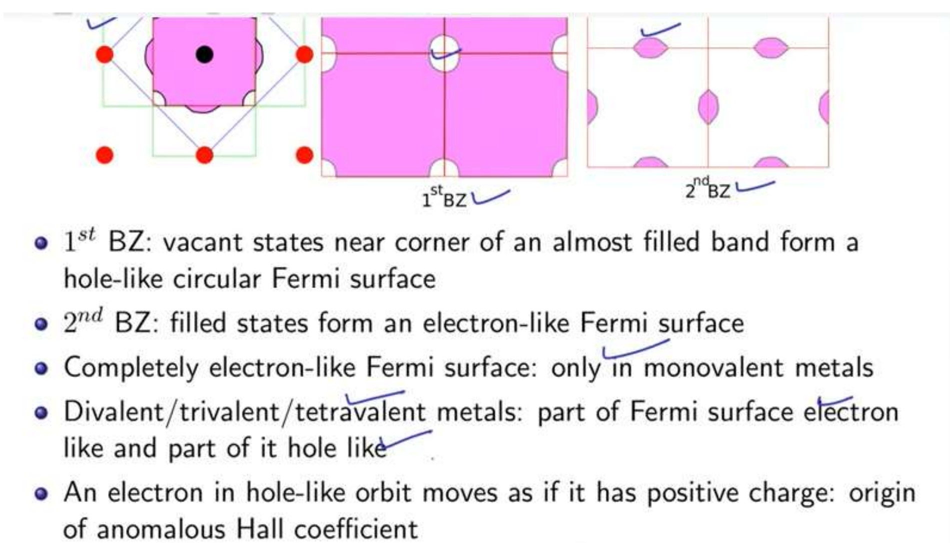

Obviously completely electron like Fermi surface can exist only in case of monovalent metals because Fermi surface does not cross the first Brillouin zone boundary in this case of divalent trivalent or tetravalent metals part of the Fermi surface is electron like and part of it is whole like. In case the Fermi surface is whole like an electron in whole like orbit moves, As if it has a positive charge this must be related to the anomalous all coefficient in divalent trivalent or tetravalent metals.

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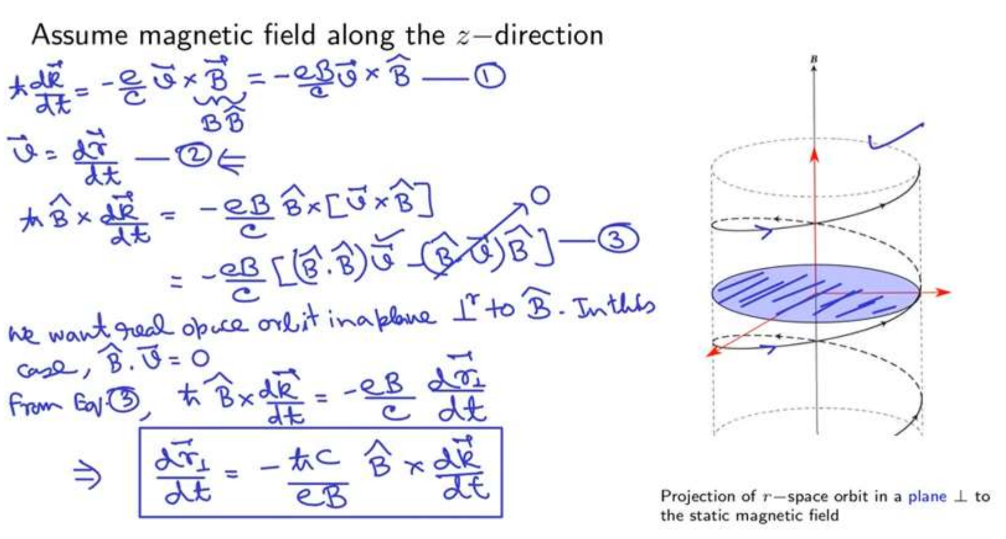

So far, we have been discussing electron orbit in the case space. Let us now discuss about electron orbit in real space in the presence of a static magnetic field equation of motion is h cross decay d t -e by c B cross d now. We express the vector d in terms Pockets magnitude and unit vector in the direction of d such that this equation is - e B divided by c v cross B hat, let me call this as equation 1.

Velocity v = d r right d t let me call this as equation 2. in equation 1 we take a cross product with B such that left hand side is part B hat cross d k d t = -e B by C B Hat cross v cross B which is equal to -e B by C B hat dot B hat – B hat dot v hat let me call this as equation 3. As shown in this diagram the blue plane is perpendicular to the direction of external magnetic field.

We want to get the projection of r space orbit which is shown by this black line in this plane which is perpendicular to the external magnetic field. Thus we want real space orbit in a plane perpendicular to B in this case B hat dot v = 0. So this term is 0 then from equation 3, we get h bar d hat cross d k d t = - e B by C. And in case of v I just write d r d t. Since R is lying in a plane which is perpendicular to the external magnetic field, I write a small subscript perpendicular.

Finally, we can write it as d r perpendicular d t = - h bar C divided by e B hat cross d k d t. Thus projection of the r space orbit in a plane perpendicular to the field can be obtained from the k space orbit.

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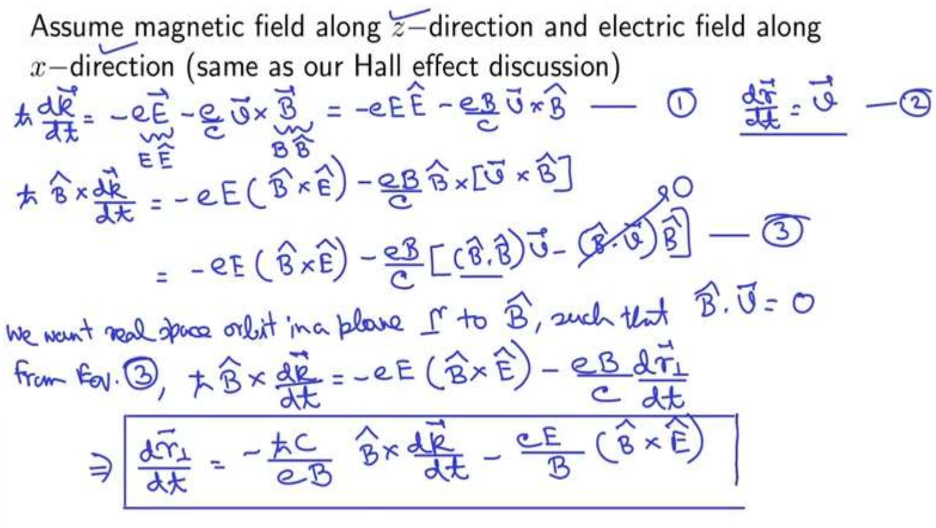

Finally solving this equation, let us apply simultaneous magnetic and electric field. Assume magnetic field along the Z direction and literary field along the X direction this is same as our Hall effect discussion. The equation of motion is h bar d k d t = -e times the electric field -e by C v cross B. Now this vector I write it as magnitude times the unit vector similarly this vector I write it as its magnitude times the unit vector.

And then we can rewrite the equation as -e times E hat - e B divided by C v cross B hat let me call this as equation 1. We know that d r d t = v I call this as equation 2. Now in equation 1 I did cross product with B handling such that the left-hand side is h cross B hat cross d k d t = -e times E B hat cross E hat –e B by C B hat cross V + B hat and this is equal to - E e D Hat Cross yet -E B by C B hat B hat D at B -B hat dot v B hat let me call this as equation 3.

Now as explained previous slide we want real space orbit in a plane perpendicular to B such that B hat dot v = 0 so this term is 0 in equation 3. Thus from equation 3 we get h bar B Hat cross d k d t = - e times E B hat Cross E hat -e B by c B hat dot b hat is 1 and in place of v I just write d r d t since r is a vector lying in a plane perpendicular to d I just write a small subscript perpendicular. Thus we get d r perpendicular d t = -h Bar C divided by e times B hat cross d k d t - C times E divided by B D hat cross E hat.

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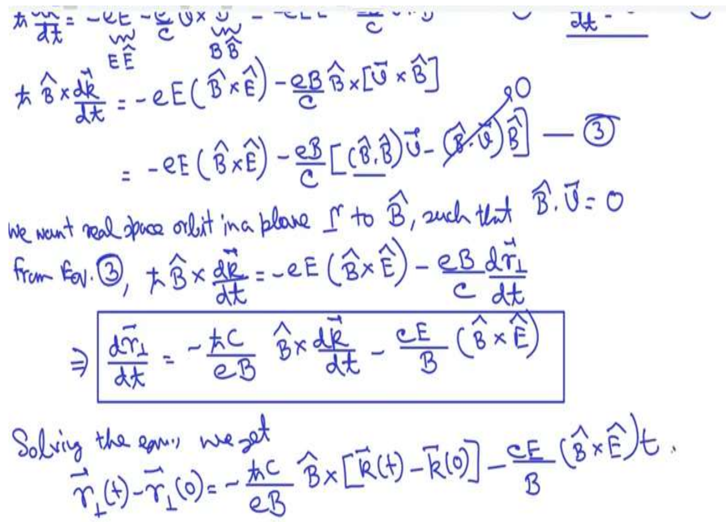

Solving this equation, we get r perpendicular at time t - r perpendicular at time 0 = - h Bar C divided by e timesB, B hat cross k of t - k of 0 - c E divided by B, B hat cross E times t.

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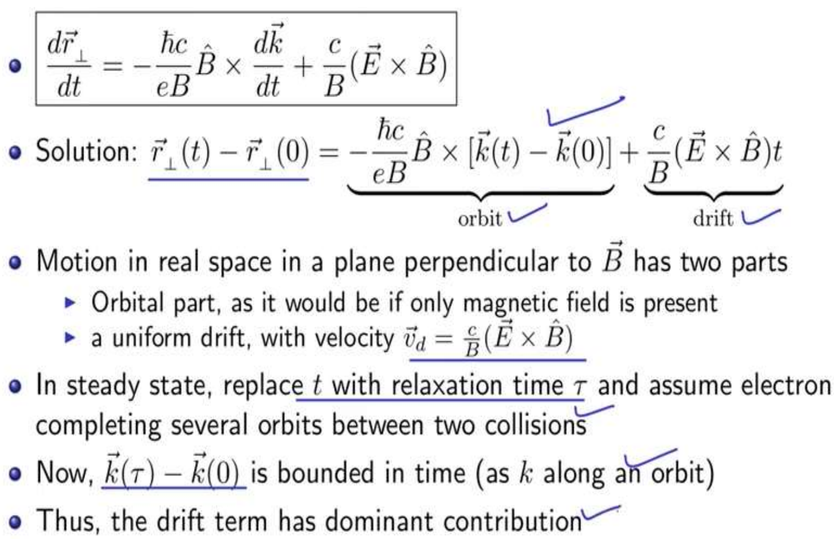

So, we are considering a case of applying uniform electric field in addition to the static magnetic field. This is how position of electron is changing in a plane perpendicular to the magnetic field. Motion has 2 parts or vital part as it would be if only magnetic field is present. In addition to the orbital part, we have a uniform drift term with drip velocity v d = c by B times electric field cross B hat.

In steady state we have to replace t with relaxation time down and we also assume that the electron is completing several orbits between 2 collisions. We know that if only magnetic field is applied the electron is doing orbital motion in case S as well. So this term is bounded in time as k is along an orbit thus the drift term has dominant contribution.

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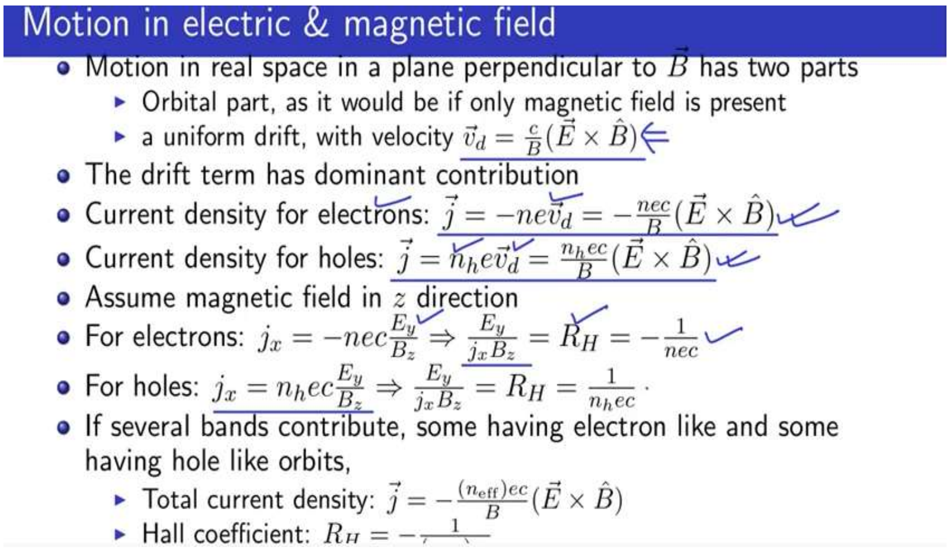

Now let us consider current density for electrons J = - n e times the drift velocity the drift velocity is given by this equation such that the current density can be written in this form. Similarly current density for holes is given by j = n h times e times v d where n h is the density of holes and e v is the drip velocity, which is given by this equation such that the current density of for holes can be written as this as you the magnetic field to be in Z direction an electric field is applied in the x Direction.

And as a result of loading slopes a transverse electric field builds up in the y direction, if we just take the x component from both sides of this equation then we get j x = - n e c times E y by B z which can be related as E y by J x B z which is equal to the whole coefficient which is equal to -1 by n e c. Similarly, by equating the x component from both sides of this equation we get j x = n h times E times c times E y by B z for holes.

Which implies that the whole coefficient for holes is given by RH = 1 by n h e c thus whole coefficient for electron and hole have opposite side.

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- Current density for electrons: $j = -ne\vec{v}_d = -\frac{nec}{B}(E \times B)$
- Current density for holes: $\vec{j} = n_h e\vec{v}_d = \frac{n_h ec}{B}(\vec{E} \times \hat{B})$
- Assume magnetic field in z direction
- For electrons: $j_x = -nec\frac{E_y}{B_z} \Rightarrow \frac{E_y}{j_x B_z} = R_H = -\frac{1}{nec}$
- For holes: $j_x = n_h ec\frac{E_y}{B_z} \Rightarrow \frac{E_y}{j_x B_z} = R_H = \frac{1}{n_h ec}$
- If several bands contribute, some having electron like and some having hole like orbits,
  - Total current density: $\vec{j} = -\frac{(n_{\text{eff}})ec}{B}(\vec{E} \times \hat{B})$
  - Hall coefficient: $R_H = -\frac{1}{(n_{\text{eff}})ec}$
  - $n_{\text{eff}} =$ total density of electrons minus total density of holes
- In case of di/tri/tetra-valent metals, part of Fermi surface is electron like and part of it is hole like
- More contribution coming from the hole like part leads to anomalous Hall coefficient

Now if several bands contribute to the current sum having electron like and some having whole like orbits. Then the total current density is given by this equation where n effective is the total density of electrons minus the total density of holes and the all coefficient is given by RH = -1 divided by an effective times e times c. In case of divalent trivalent or intravalent Metals part of the Fermi surface is electrolyte and part of it is whole life. If more contribution is coming from the whole like Fermi surface then that leads to anomalous Hall coefficient.