Electronic Properties of the Materials: Computational Approach
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Module No # 07
Lecture No # 31
Semi Classical Electron Dynamics: Concept of Hole

Hello friends we have derived the governing equations of semi-classical electron dynamics and discussed about the limits of semi-classical model in detail. We have found that compared to the free electrons velocity of block electrons differ particularly for the electrons with wave vector close to the zone boundary. In this lecture i am going to introduce a very important concept of whole. Concept of whole is a remarkable achievement of the semi-classical model which can give satisfactory explanation for anomalous all coefficient in some metals.

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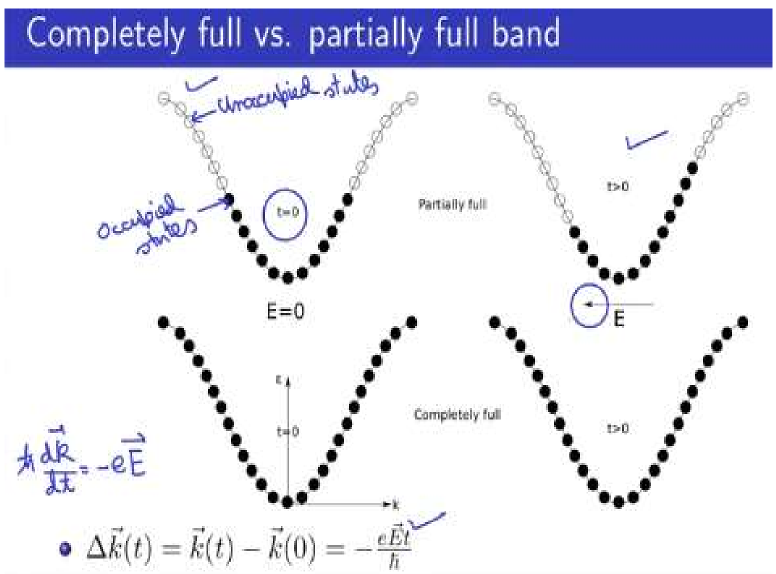

First let me show that a completely full band does not take part in electronic transport by using some simple arguments. We apply an external electric field and solve the equation of motion $\hbar \frac{d\vec{k}}{dt} = -e\vec{E}$ we have to find how k is changing as a function of time and this is how the k changes as a function of time.

Let us imagine that we have a partially full band in this diagram we are open circles represent on occupied states. And field circles represent occupied states this is how the states are occupied at p

= 0. Now at this point of time we switch on at electric field in this direction this is how the occupation of the state changes when we switch on the electric field. Note that before applying the field equal numbers of positive and negative k points were occupied after applying the field more number of positive k points is occupied.

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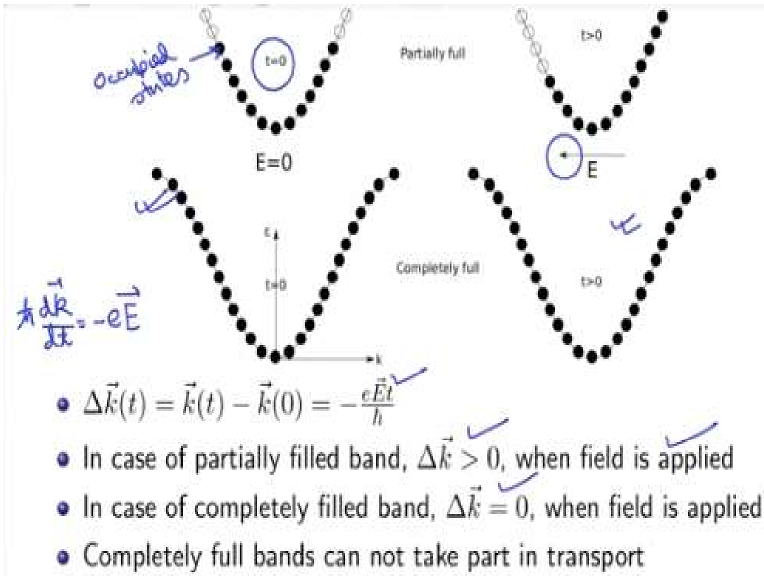

As a result net change of k is positive when field is applied in this particular direction. Now let us consider the case of a completely filled band in this case delta k = 0 even in finite electric field as shown here. As a result we cannot get any current in case of a completely full band in conclusion completely full bands cannot take part in transport process.

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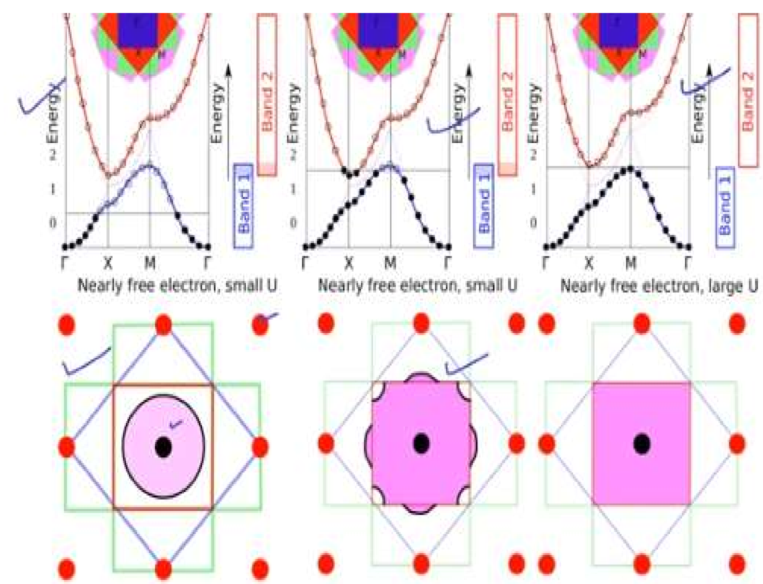

So far our discussion is based on 1d cartoons let us look at some more realistic picture. This is how the partially field bands of monovalent atoms look like in case of a monovalent metal. I have assumed a 2d square lattice this is how it looks like if we draw the corresponding constant energy fermi surface in reciprocal space. The Fermi surface is circular the magenta shaded region is the field portion of the reciprocal space.

The black point in the center is the gamma point and the red points are adjacent reciprocal lattice points. The third diagram shows a divalent solid with some band camp as a result the first band is completely full and the second band is completely empty this is an insulator. The second diagram is a divalent metal where both first and second band is partially full because of band overlap Fermi surface is fragmented part of it lying in the first Brillouin zone and part of it in the second Brillouin zone.

Electrons in the first and second solid will take part in transport process because of partially full bands. In case of the third solid electrons cannot take part in transport process because of the completely full band. Transport is possible if we can excite some electrons from the first band to the second band in some way for example via thermal excitation.

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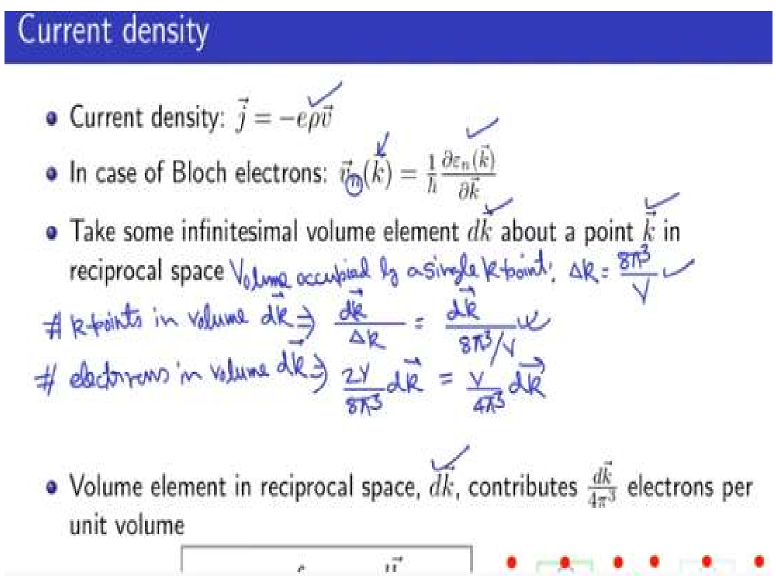

Let us derive the expression of current density of block electrons we start with the regular expression of current density given by j = - e times; rho time’s b - e is the charge of electron which is a fundamental constant so rho is the radial density and b is the velocity. We have to determine rho and v for block electrons velocity is given by the first derivative of energy with respect to k.

Note that velocity depends on k as well as on the band index n there is no simple explicit expression for energy of block electrons as a result there is no simple explicit expression for velocity as well. Now let us try to get the electron density rho of block electrons we know that

Volume occupied by a single k-point $\Delta k = \frac{8\pi^3}{V}$where V is the volume of the solid

Now consider a volume d k about a point k in the reciprocal space.

Number of k-points in volume $d\vec{k} \Rightarrow \frac{d\vec{k}}{\Delta k} = \frac{d\vec{k}}{8\pi^3/V}$

Now each k-point can hold up to 2 electrons according to Pauli's extinction principle thus to get the number of electrons in volume d k we have to just take this number and multiply it with 2. And we get $\frac{2V}{8\pi^3}d\vec{k} = \frac{V}{4\pi^3}d\vec{k}$. Thus, infinitesimal volume element in reciprocal space d k contributes d k divided by 4 phi cube electrons per unit volume.

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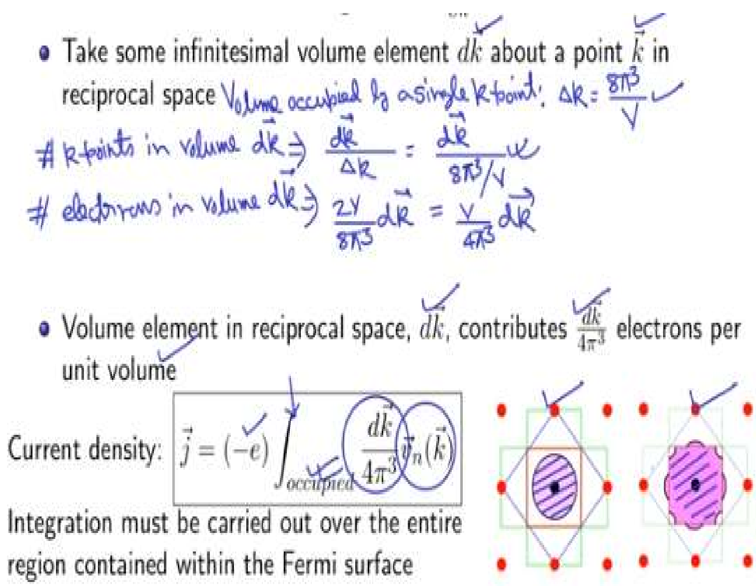

Now current density is -e which is the charge of an electron times d k divided by 4 phi cube which is the number of electrons per unit volume types v of k which is the velocity of electrons. We have to integrate over the occupied states let us try to understand what do we mean by integration over the occupied states. This implies that integration needs to be carried out over the entire region content within the Fermi surface.

For example in this case over the entire Fermi circle as shown by this hashed area on the other hand in case of the second figure integration needs to be carried out over the entire fragmented region part of which is lying in the first Brillouin zone and part of which is lying in the second Brillouin zone.

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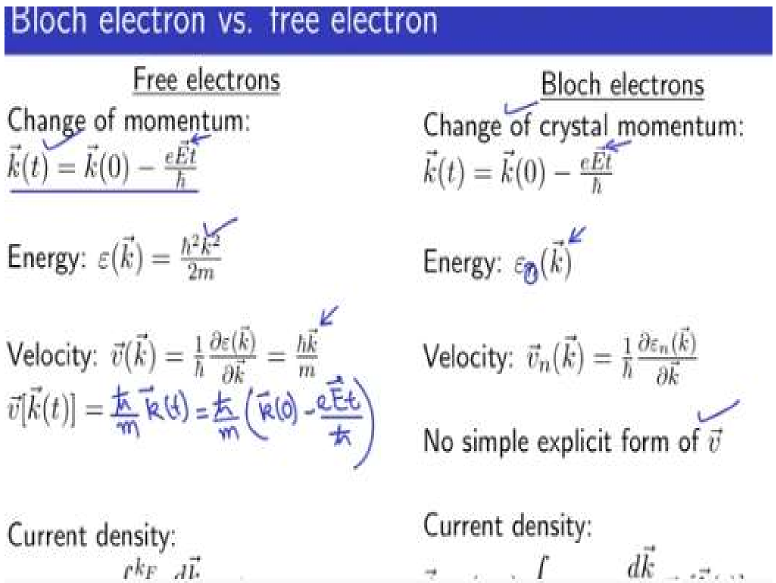

Before proceeding further let me compare the steps leading to current density calculation for block and free electrons side by side. In case of free electrons this is how momentum changes when an external electric field is applied and this is how the crystal momentum changes in case of a block electron when an external electric field is applied. Energy of free electron depend quadratic on wave vector k.

For block electrons there is no simple explicit form energy depends on k as well as the band index n in case of free electrons velocity depends linearly on point vector t. As a result we have a simple expression for velocity at time t given by h cross by m time's k t; that we get k from this equation such that velocity at time t is h cross by m k 0 - E t by h. In case of block electrons we do not have any simple explicit form of velocity. Velocity has to be calculated from the first derivative of energy with respect to the wave factor.

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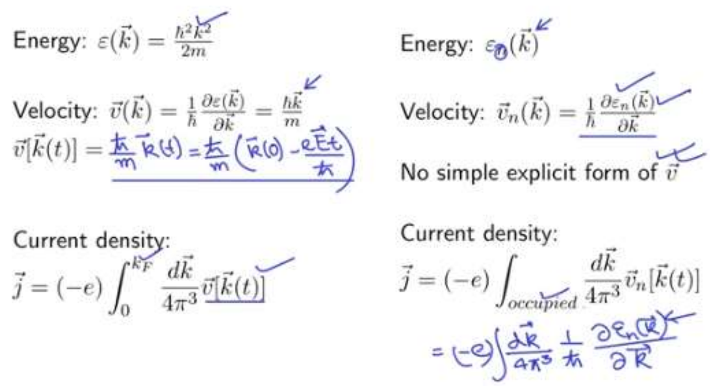

Finally the current density is obtained by integrating v in case s over the Fermi sphere of radius f. Since we know the exact form of v from this equation we can easily evaluate this integral in case of block electrons there is no simple explicit form of v. V is obtained from the first derivative of energy with respect to k; thus the expression for current is -e integral d k by 4 phi cube. Since we do not have any simple explicit form we have to use this 1 by h bar del e divided by then thus current which depend on the energy dispersion relation of block electrons.

In this case the Fermi surface need not be spherical thus we have to carry out the integration of v over the occupied region in reciprocal space the occupied region need not be spherical it can have some very complicated shape.

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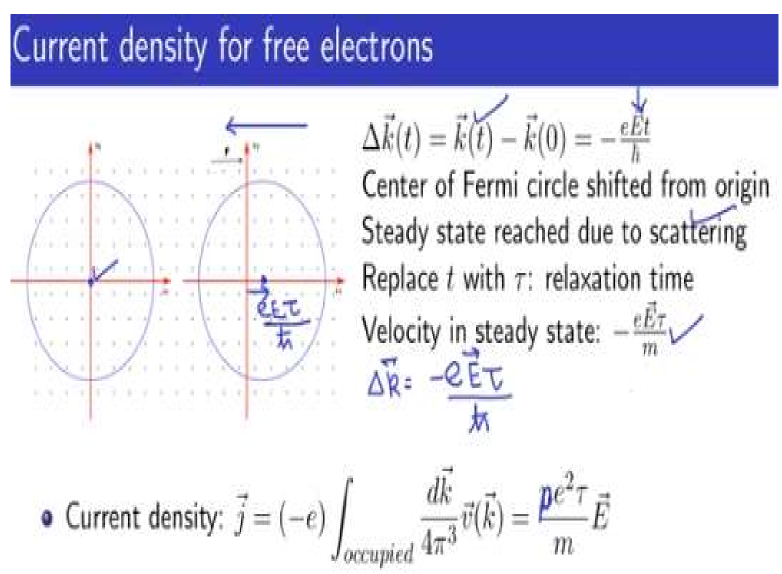

Let us first try to get the current density of free electrons this is how k changes when we apply an electric field e. When electric field is 0 Fermi circle is centered at the origin of the k space when an external electric field is applied in this direction center of the Fermi circle is shifted from the origin of the k space. From the equation you may conclude that the center of the Fermi circle keeps shifting towards the right as long as the field is on.

However that does not happen because steady state is attained very soon due to scattering thus we replace t with a constant tau which is also known as the relaxation time. Thus in the steady state delta k = -e times electric field times tau divided by h bar. From this we get the steady state velocity as - e times electric field time's tau divided by m.

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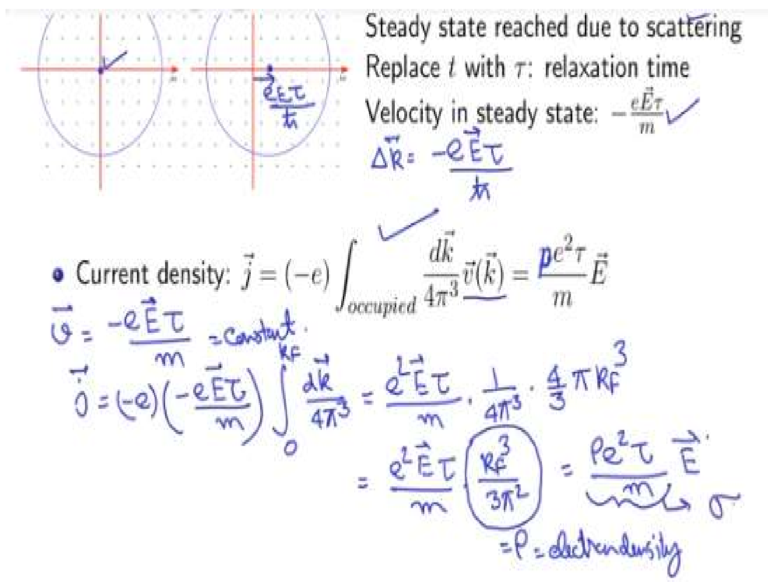

Now let us find the current density by evaluating this integral note that the velocity v is a constant; which is equal to charge of the electrons times the electric field time's relaxation time divided by mass.

$$\vec{v} = \frac{-e\vec{E}\tau}{m} = \text{constant}$$

Since these are constant let us bring v out of the integer and rewrite j

$$\vec{j} = -e\frac{-e\vec{E}\tau}{m}\int_0^{k_F}\frac{d\vec{k}}{4\pi^3}$$

Note that the integral is over a Fermi circle of radius k f such that we can put the limit as 0 to k. Integral 0 to k f d k must be equal to the volume of a sphere of radius k f in k space. Such that we can write j s e square times electric field times tau divided by m into 1 by 4 phi cube into volume of the sphere with radius k f

$$= \frac{e^2 \vec{E} \tau}{m} \frac{1}{4\pi^3} \frac{4}{3} \pi k_F^3$$

and this is equal to e square times electric field tau divided by m times k f cube divided by 3 phi square.

$$= \frac{e^2 \vec{E} \tau}{m} \frac{k_F^3}{3\pi^2}$$

Note that this term is equal to rho the electron density thus we can rewrite this equation as rho times e square times tau divided by m times the electric field where this term rho e square tau by m is the electrical conductivity sigma.

$$= \frac{\rho e^2 \tau}{m} \vec{E}$$

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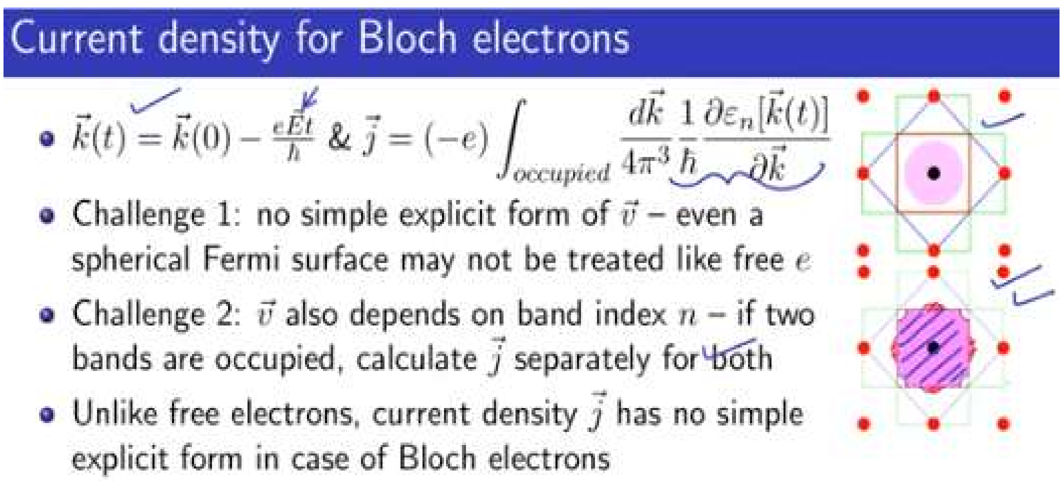

Now let us calculate current density for block electrons this is not as simple as free electrons and I want to highlight the difficulties very clearly in this slide this is how crystal momentum changes when we apply an electric field e. We have to evaluate the integral of velocity over the occupied portion of the reciprocal space to get the current density this is where the calculation differs from free electrons.

Let us first consider a partially full band such that we have a nice circular free electron like Fermi surface as shown here you may think that at least in this case we can easily evaluate the integral like we did for free electrons however it is not necessarily true. Remember that in case of free electrons velocity is a linear function of k as a result it is not too difficult to evaluate the integral to find j.

However in case of block electrons there is no simple explicit form of v; thus we have to always calculate b from the first derivatives of energy with respect to k. As a result even if we have a free electron like Fermi surface we may not be able to treat the problem as a free electron problem. In case the Fermi surface extends beyond the first Brillouin zone it becomes even more difficult. For example in this case both the first and second band is partial occupied velocity also depends on band index n.

As a result we have to calculate j separately for both the bands. For example when we evaluate the integral of v k over the occupied regions in the first Brillouin zone then we get the current from the first band. And when we integrate v k over the occupied regions in the second Brillouin zone then we get the current from the second band. In conclusion unlike free electrons current density has no simple explicit form in case of block electrons.

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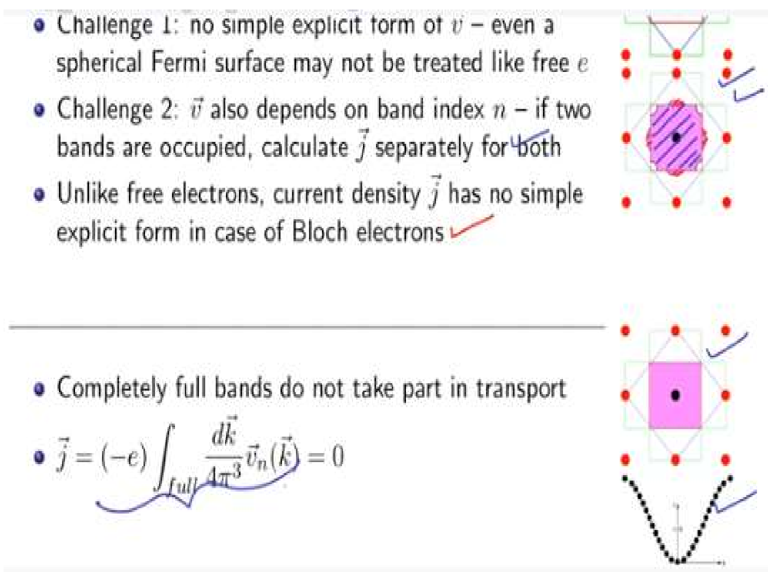

Now let us look at the most important message we can carry forward from this slide. This is a completely full band there is no band overlap. In k space the first Brillouin zone is completely occupied and rest of the Brillouin zone are unoccupied. We know that completely full bands do not take part in transport as a result if we evaluate this integral over the full Brillouin zone we should get 0.

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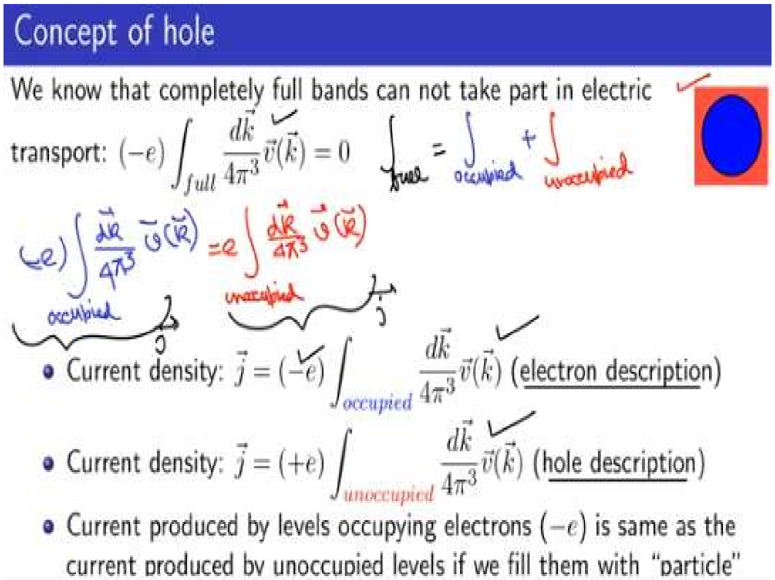

Based on our discussion so far let me introduce a very important concept, concept of whole. We already know that completely full bands cannot take part in electric transport and if we carry out this integral over the entire Brillouin zone which represents a full band we get 0. Now let us split the integral over the full Brillouin zone into 2 parts integral over the occupied region plus integral over the unoccupied region.

That is for example let us consider a simple case where we have a free electron light Fermi surface the blue region of the very Brillouin zone is occupied and the red region of the Brillouin zone is unoccupied. Splitting the integral over full body language zone into 2 parts we get -e integral over occupied and integral over unoccupied and this should be equal to 0. Now we can rewrite this equation by bringing the integral over unoccupied states to the right hand side.

Such that we can just write it as this since the left hand side is equal to j the right hand side also has to be equal to j the correct density. Thus current density can either be obtained by calculating this integral over the occupied states or by calculating this integral over the unoccupied states. The first one is known as the electron description as the charge carrier is negative the second one is the hole description because if you note carefully in this equation the charge area is positive.

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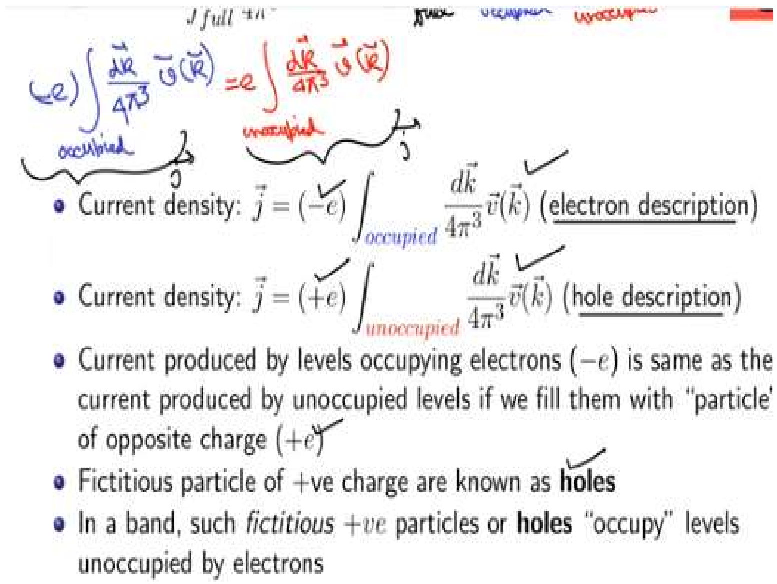

In conclusion current produced by levels occupy electrons of charge -e is same as the current produced by unoccupied levels if we fill them with particle of opposite charge that is +e. Remember that only charge carriers are electrons however sometimes it is more convenient to describe the current to be carried by fictitious particles of positive charge known as holes. In a band such fictitious positively charged particles or holes occupy the levels unoccupied by electrons.