Semiconductor Device Modeling
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Lecture - 13
Semi-classical Bulk Transport: EM Field and Transport Equations

In the previous lecture, we discussed a solution of the BT by imagination and substitution. We talked about Displaced-Maxwellian Approximation for the distribution function f. We showed how this approximation can be developed from the solution under equilibrium. The Boltzmann Transport Equation gets considerably simplified under equilibrium and it can be shown that the Fermi-Dirac distribution function is a solution of the Boltzmann Transport Equation under equilibrium provided the Fermi level.

And the lattice temperatures are assumed to be constant throughout the device. We also gave formulae for the carrier concentration and current density in terms of Displaced-Maxwellian Approximation. So, we said that the form of the Displaced-Maxwellian Approximation is developed, by looking at the equilibrium Fermi-Dirac distribution approximating it by Maxwell Boltzmann distribution.

And then incorporating in the equilibrium Maxwell Boltzmann distribution. The presence of directed component of velocity or non 0 momentum and a carrier temperature different from lattice temperature. So, these 2 things we incorporate in the equilibrium Maxwell Boltzmann distribution to get the Displaced-Maxwellian Approximation. We also introduced an alternate approach to use the Boltzmann Transport Equation to get the carrier concentration and current density.

Now, let us develop the second approach in more detail here.

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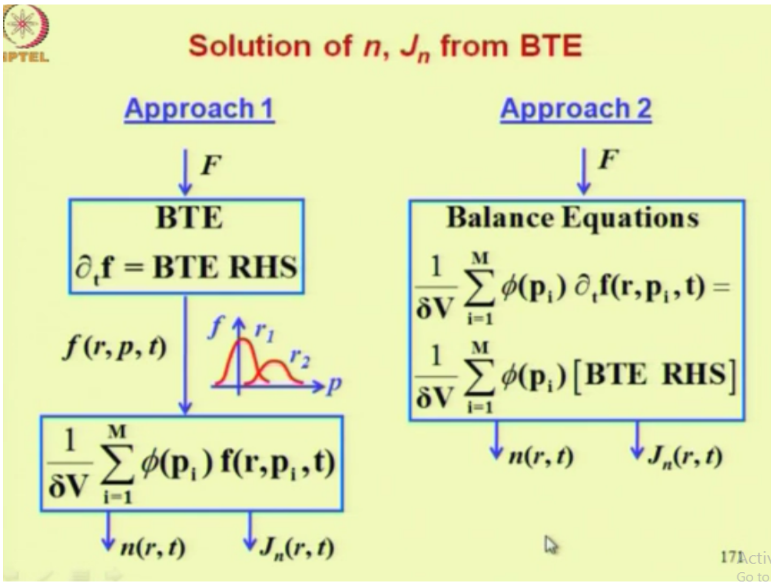

So, the first approach let us summarize in the form of a block diagram. You have the Boltzmann Transport Equation which is shown here as dou f/dou T equal to the right hand side terms of the Boltzmann Transport Equation. The input to this equation is the force on an electron. This is obtained from solution of the Maxwell's equations. Output of the Boltzmann Transport Equation is the distribution function f (r, p, t).

So, in general this distribution functions the expression for this is a function of 7 variables x, y, z which is shown here by the symbol r, Px, Py, Pz which is shown here by the symbol p and t. So, the 7 variable function is rather difficult to solve for, okay. Anyway, if you have these solutions somehow then you can use this solution and substitute it in this formulae to get the carrier concentration n and the carrier current density Jn.

This n and Jn are functions of position and time only. So, the momentum term has gone out of the expression because these expressions are derived using the formulae here in which you are summing up some expression over all momentum states. So, in that process the momentum information has been already incorporated. Let us look at this equation, phi is a function of p by choosing an appropriate function of p you get n or Jn.

For example, if you choose phi of Pi = 1 then the formula = n. If you choose phi of Pi = -q times p/Mn then you get Jn. This formula we are given in the previous lecture. Now because this 7 variable function is difficult to obtain for a general situation the Displaced-Maxwellian Approximation was a case of inspired guess trying to anticipate the form of the solution and check whether the solution works. Now unfortunately the solution for Displaced-Maxwellian Approximation may not work for all cases.

That is the difficulty. So, now what is alternate approach? We exploit the fact that what we are interested in is n and Jn and here you really do not need the momentum information ultimately. It does not appear in these expressions. Now that being the case can we not perform this operation of multiplication of the distribution function by the function phi and then summing out over the states on the Boltzmann Transport Equation itself.

So, rather than getting f and then performing this operation, why not we shift this operation into the equation itself? So, that is the approach that we in introduced in the previous lecture. Now this is shown in the block diagram and the resulting equations are called balance equations. So, you can see what we are doing is that we are multiplying all the terms of this equation by phi and then summing up over all the states all the momentum states.

With the result that the left hand side of the Boltzmann Transport Equation becomes a function of either n, Jn or other such quantities. For example, if phi of Pi is 1 then the left hand side this term becomes dou of n/dou t. If we choose phi of Pi as Pi/QMn then it becomes dou Jn/dou t. So, this term becomes dou Jn/dou t and this we showed in the previous lecture by doing a simple derivation.

Now we would like to develop this approach in more detail to get all the other terms of these balance equations mainly what are the terms on the right hand side.

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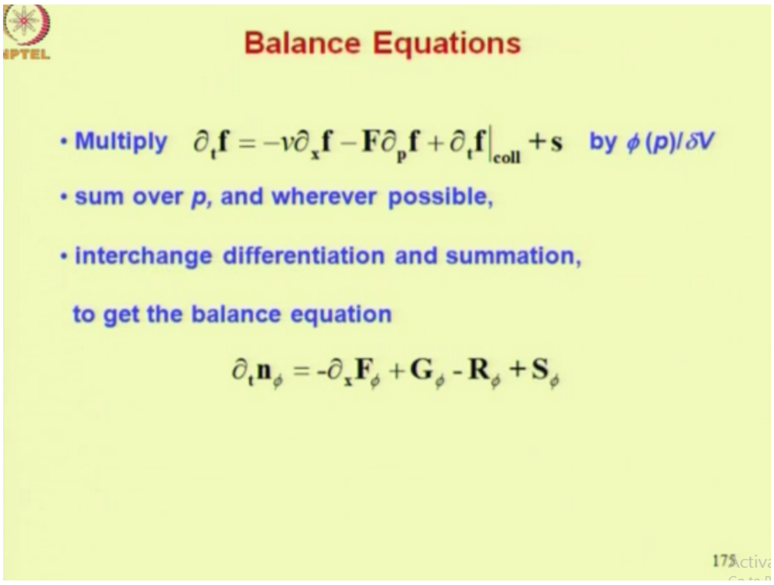

So here before we set out to do that since we have some number of mathematical derivations. Let us put down the steps. So, you take the Boltzmann Transport Equation multiply by phi p/delta V. Then you sum over all the momentum states p and this is important wherever possible interchange differentiation and summation. So, this is the step that we should particularly take note off. The result will be you will get a balance equation like this.

So, here each term corresponds to the, a term of the Boltzmann Transport Equation. So, dou of n phi/dou t corresponds to dou f/dou T - dou/dou x of F phi corresponds to –v into dou/dou x of f. G phi corresponds to –F dou p. R phi corresponds to dou phi dou t of f due to collisions with an appropriate sign of course and S phi corresponds to the term S.

So, each of these terms after manipulation as suggested here, namely multiplication by phi p/delta V summation over p and interchange of differentiation and summation will result in these terms. So, let us derive the expression for various terms of this balance equation in terms of phi p and the terms of the Boltzmann transport Equation.

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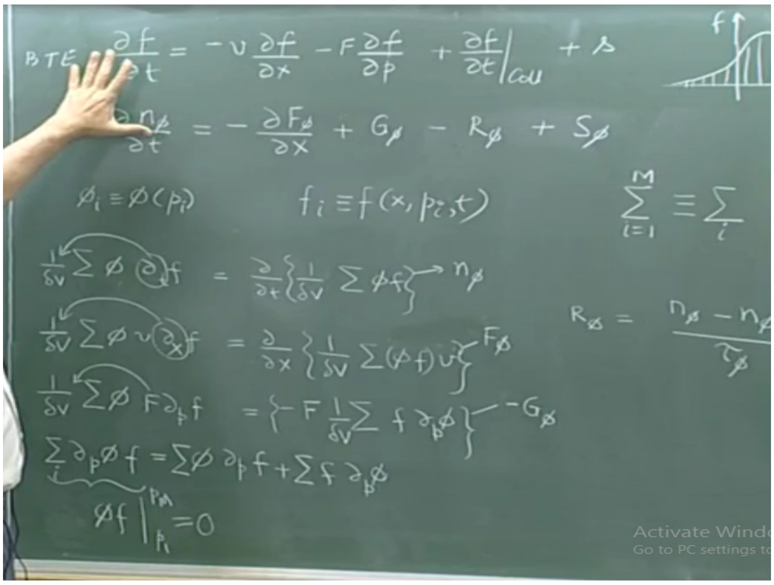

So, here we have written the BTE. Now when we go through since, we have a number of terms to be written in an equation we would like the notation to be compact, so here I have shown some abbreviation. So, phi of Pi will be represented as phi i, f of x, Pi, t will be represented as fi and the summation I = 1 to M will represented as simply summation i. Phi of p will be simply represented as phi and f of x Pt will be f, okay.

So, now let us take this term and derive the n phi we have done it in the previous lecture I will just quickly put the result. So, multiply by phi then sum and divide by delta V that is why this n phi is. So, when you are summing over phi. Now this is where we do interchanging of differentiation and summation since phi is a function of P, I can always move the time derivative out. So, I can push it out here phi is not a function of time and the result will be this, okay.

Now this can be actually written as and that is what here n phi is. So, since we will use this expression later on to derive specific expressions for balance equations, so we will put this here.

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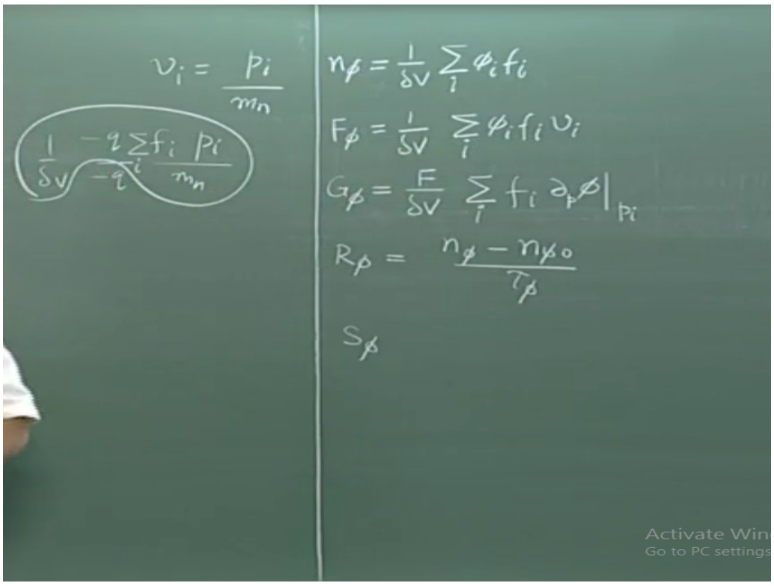

So n phi is equal to this. Now, let us look at the next term F phi. What is f phi? So, let us operate on this phi into V into dou/dou f of x delta V. Now the velocity V is a function of p it is not a function of x. Phi is a function of p not a function of x. So I can shift like I shifted dou/dou t here, I can shift dou/dou x again out here and my result will be dou/dou x, 1/delta V into f, v, phi.

What we will do is we will shift this v to the end recognize that the term phi into v into f is phi into f into v and therefore this is flux of this quantity phi f, V is the velocity. Now in this expression you had phi into f, so this term was n phi. You can see that this term can be now called the flux of n phi. That is why the symbol F phi. So, not just this actually, this whole thing within flower brackets, okay. So, this is the expression for your F phi here.

So, let us write that down F phi = 1/delta V sigma i. Now let u take the third term. So, again multiply by phi and you have f dou/dou P of f sigma delta v here derived. Now unlike the earlier cases phi is now a function of P, please note here. Therefore, I cannot move this dou/dou P sign out very easily. I cannot just push this phi inside. However, the force F depends on the electric filed E and it is not a function of P.

For example, f is = -q times E. Therefore, I can push the f in but not phi. So what do we do here? So, first let us push the f out at least. So, that this goes out and we have to deal with phi into dou/dou f of P. Now note that if I take phi into f both of which depend on P and perform the differentiation operation then this will be phi into this +f into derivative of phi with respect to P.

Now derivative of phi with respect to P can be easily derived because phi is a function of P and therefore what we do is we write this quantity phi into dou P/dou f which is what has come here as difference between this quantity and this quantity. Now you will say but what is the advantage of converting one expression into 2 expressions. You do realize that phi is a function of P alone and therefore this can be derived very easily but what about this?

Well, as we will show shortly, when you do a summation of this quantity over all the states ultimately you have done the summation this quantity will simple become 0. So, let us write that down. So, if I now do a summation I have to sum over all the states i. Now if you know the distribution function it looks something like this. This is the P axis and this is the f. Now if you take all the states your states will extent from P = t - infinity to P =+infinity in principle.

So, all these, these all your states, allowed states. Now you see differentiation and summation is nothing but it is analog us to integrating the differential and therefore this quantity is nothing but phi of f. The 2 limits being the one extreme state i and the other extreme state. So, P1 to pm suppose we said there are m states, so P corresponding to P1 and Pm.

Now, since the number of states is large and they extent from - infinity to + infinity that is what we have said. So, P1 may be somewhere here and Pm maybe somewhere there. So the function f has dropped to 0. So, no matter what your phi is both this limits this quantity will be 0 and therefore this is equal to 0 Now that is advantage, so you have converted this expression into a simpler expression. So, if you do that write that down now use this pack.

So this will turn out to be F into sigma, capital F into sigma small f into dou/dou f of P. Now note this is 0 and we want this expression so this will be -. There will be a negative sign here and you have 1/delta V term. So this is your, this whole quantity is your - of G phi. Why is it - because you see - of f dou f/dou P has been put as G phi, okay? So, this quantity alone if you see it is - of G phi.

So therefore I can, if I remove the negative sign here and I can put these 2 negative signs together and then remove the negative signs and let me write the resulting expression here. So, G phi = 1/delta V summing over all the states fi dou f/dou P corresponding to Pi into the force F here, okay. So, that is what your G phi is. R phi, now you recall we have remarked that this quantity and this quantity these 2 have to be derived from Quantum mechanics, okay?

So, we are not going to do much of a derivation regarding these. We will simply assume a form that is commonly used, okay. So, R phi for example is commonly cast in the form n phi - n phi under equilibrium by a time constant dou phi. n phi is the, this quantity n phi that is this quantity, right, obtained from f by multiplication by phi summation and all that. This form is dictated by for example our familiarity with the recombination expression, right.

You recall you want to write down an expression for recombination rate of carriers, of minority carriers you write the recombination rate as minority carrier concentration - the equilibrium minority carrier concentration by the time constant associated with the recombination. Now that is the kind of motivation for writing this form. So, the dou phi here will be derived from Quantum mechanics.

You can always write, you can multiply dou f/dou T/phi, do summation and so on. Now that expression I will not write here, I will write only the final result, okay. But let us interpret what this result means, so dou phi is a time constant that tells you how the quantity n phi will be driven towards equilibrium at what rate okay that is what this dou phi means. So, let us put down this expression here. R phi = n phi.

Now a clarification here dou phi represents the rate at which n phi is driven towards equilibrium n phi 0, but by what process it is very important. The process is scattering, okay, this important. So, look at this, this dou f/dou T collision, right. Therefore, it is a collision which are responsible for pushing n phi towards equilibrium. So, the dou phi should be interpreted.

As the time constant that characterizes the drive for the quantity n phi towards equilibrium due to collisions. This is important. Similarly, this S phi we will simply retain as S phi you can always write it in terms of the S multiply by phi and then sum, right but we will retain this quantity as just S phi. So, here let me write that. We can always physically interpret this as due to electron-hole pair generation recombination process.

That physical interpretation will be sufficient for us to write this expression for the write an expression for this in different conditions. Now once we have derived these expressions for the various terms of the balance equation. You should recognize the similarity of the form of this equation to the whole continuity equation. Just like we showed the similarity of the form of this equation to whole continuity equation you should recognize the similarity.

Well, you have a time derivative of a quantity on the left hand side. You have negative of the special derivative of the flux of this quantity on the right hand side and you have some source and sink terms. Because in these equation you have a change in the quantity because of collisions as well as because of generation recombination process you have multiple terms source and sink term.

So, these 2 are the terms which are coming up because of momentum changes and this is the term that is coming up because of generation recombination processes. So, you see G phi is a generation of n phi due to the force. You can see that the G phi expression here contains the force. So, when you apply the force this force creates momentum, it generates momentum that is why these called a generation term.

Now let us interpret these terms physically, so that we will be able to use the expressions and the terms to write down balance equations for carrier concentration current density and other quantities like kinetic energy density.

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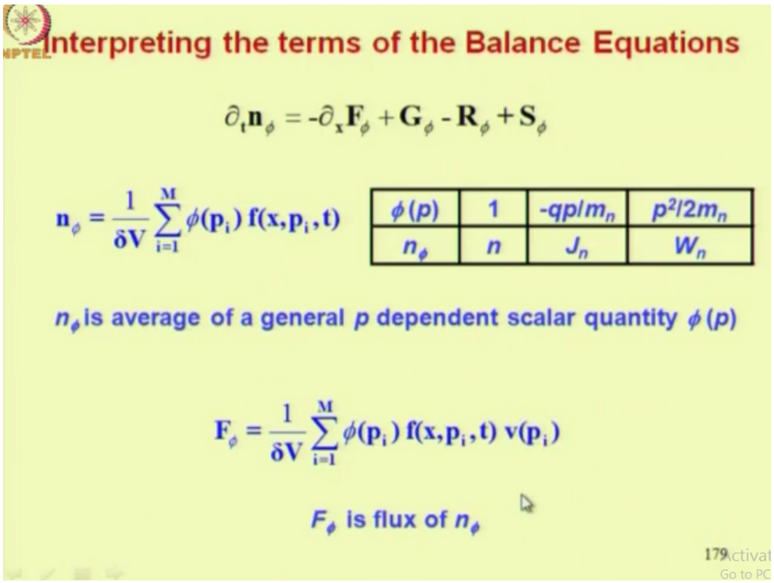

Let us start with the interpretation of n phi. So, here is the formula for n phi, n phi is the average of a general P dependent scalar quantity, phi P. So, to give you more concrete ideas let us choose some phi P's and see physically what this n phi is. This is what is represented here in the table. If we chose phi P as 1 then the formula shown here for n phi reduces to that of the carrier concentration n.

In the previous lecture we have already introduced that formula. If you multiply if you choose phi of P as -q times P/Mn then you get Jn the N phi becomes the current density Jn this also we have explained in the previous lecture the formula for Jn and similarly, if you choose phi P as P square/2Mn kinetic energy. Then you get the average kinetic energy density Wn out of this formula.

This formula for Wn was also given in the previous lecture. Now F phi is a flux of n phi because you have the velocity term here and this quantity here is the same quantity that enters in the n phi expression.

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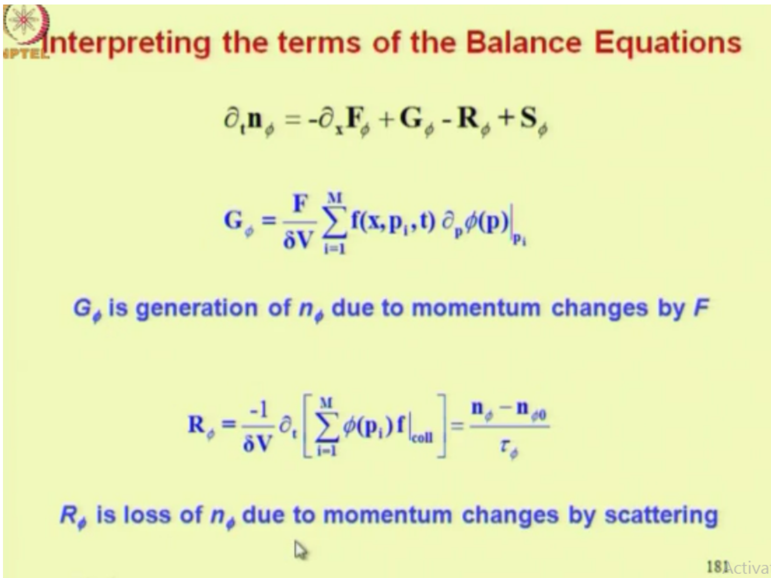

G phi is generation of n phi due to momentum changes by F. So, the applied force changes the momentum between collisions. It increases the momentum that is why it is a generation term. R phi which is expressed here I did not write this on the board because we said we will work with its simpler and more physical form. N phi -n phi 0/dou phi. So, R phi is loss of n phi due to momentum changes by scattering.

So, the scattering processes normally result in loss of momentum. So, R phi can be seen as counter part of G phi.

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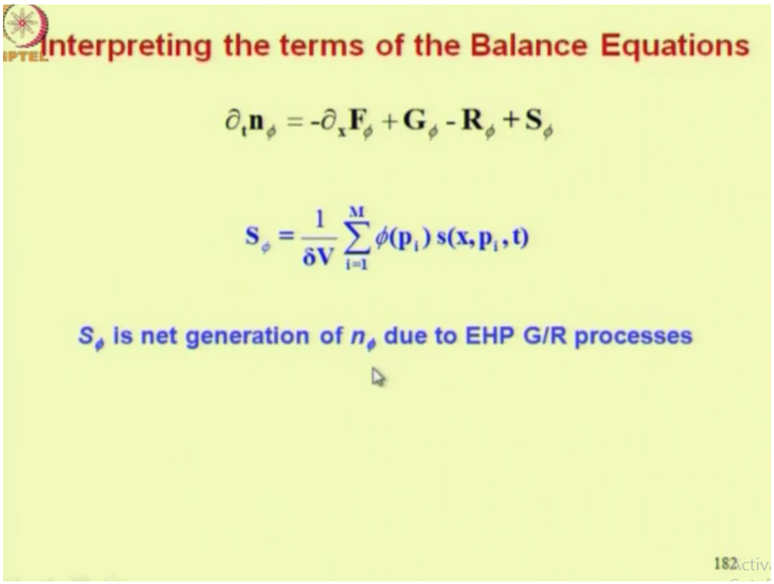

S phi, this expression also I did not write on the board because we said we will directly work with the physical interpretation of S phi. It is the net generation of n phi due to electron-hole pair generation recombination processes. Now I want to just caution you, do not think that n phi is anything to do with concentration alone, right because concentration has a symbol n and here you have n suffix phi.

So, you are likely to have that misconception but we are clearly shown that depending on what you choose for phi your n phi is different. So, if you choose phi as 1 then n phi is n, carrier concentration. Buy if you choose phi for example as P square/2Mn then n phi represents the kinetic energy density and so on, right. So, this you must bear in mind.

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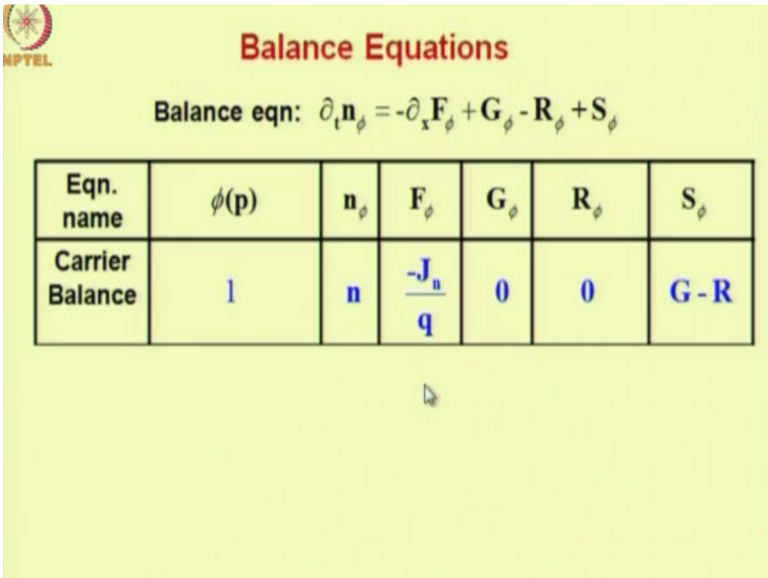

Now, let us write the balance equations for various phi P's because we want to write the equation that will give us the carrier concentration n the current density Jn. Now that is the motivation for choosing various values of various expressions for phi P and writing the expressions balance equations so that this will give us n and Jn. So, if I want an expression for n, for example, I will choose phi P as 1 and the resulting expression would be called carrier balance expression because n phi becomes n.

Now this we know already. Now F phi becomes –Jn/q. Now let us look at this point. How does F phi becomes –Jn/q, if you put phi P = 1.

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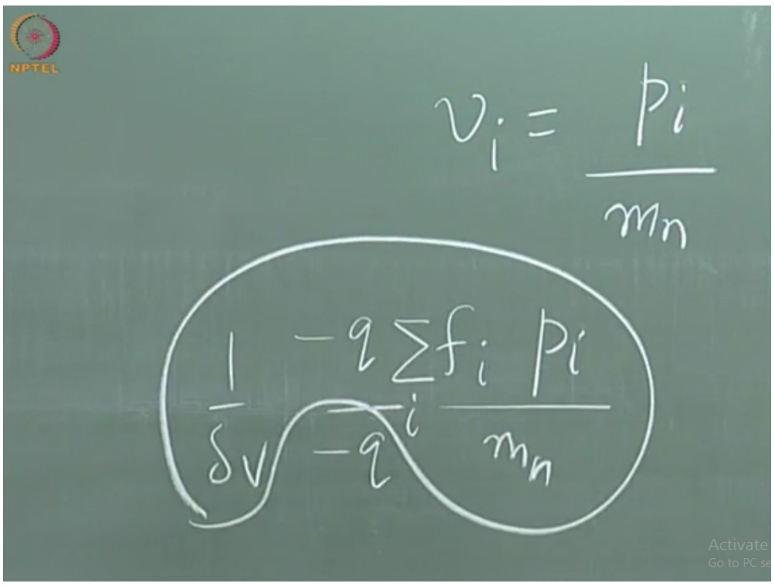

Now this is your F phi, so phi i is 1, so you have removed this. So, what you are left with is f i, Vi and VI is nothing but momentum Pi/Mn. So, here this quantity is fi into Pi/Mn. If I multiply it by -q and divide by -q then you can recognize that summing over all i and dividing by delta v. This was the formula for Jn we have derived in the previous course, our previous lecture and therefore you can recognize this to be –Jn/q.

Now look at G phi. Why is G phi 0? And why is R phi 0? Well, one way to appreciate this fact is from the physical interpretation. So, we said G phi is generation of n phi due to momentum changes by F. Now, n phi is a carrier concentration. Now is the carrier concentration changing because of the applied force? No, we are looking at a situation where the applied force does not change the carrier concentration, okay

and therefore there is no G phi there is no generation. So, another way of looking that, looking at that mathematically is your phi is 1, therefore when you differentiate it with respect to P you get 0 and that is why G phi goes to 0. Look at R phi, R phi is the loss of the quantity n phi because of momentum changes due to scattering. Now we are looking at a situation where our scattering does not change carrier concentration, okay.

Scattering changes momentum but not carrier concentration. So, evidently our phi will be 0. Another way of looking at this result would be T phi, tau phi is infinity, why because tau phi represents how the carrier concentration n is driven towards equilibrium by momentum changes. Now momentum scattering, momentum changes due to scattering do not change the carrier concentration at all that means tau phi is infinity.

The system takes infinite time to relax because it does not change at all. Finally, S phi is nothing but generation - recombination processes. This is again clear from the physical interpretation of S phi that it is generation net generation of the quantity n phi because of electron-hole per generation recombination process. So that is your carrier balance equation in the first level course.

You would have recognized based on what we have done in the first level course, you will recognize this equation to be the continuity equation. So, let me write that down.

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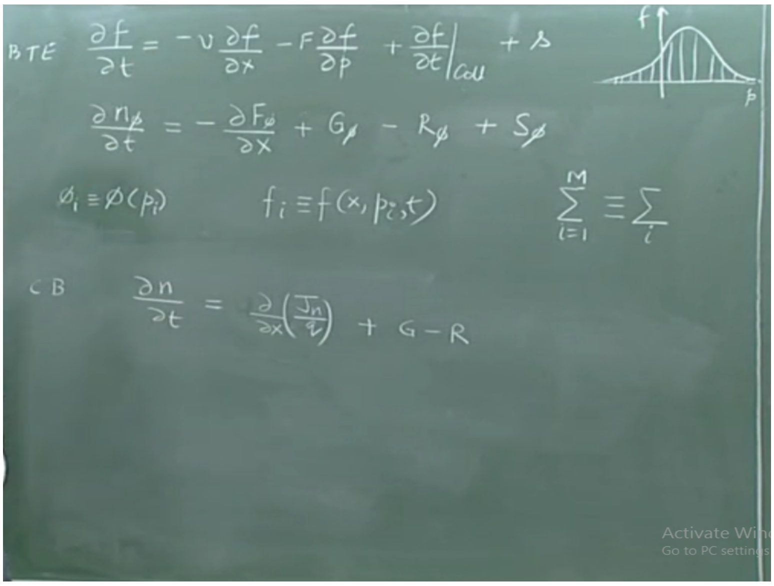

So, the carrier balance equation, let us call it as CB is dou n/dou t equal to, I think this would be a better place for write it. Dou n/dou t = -dou/dou x into Jn/-q, so these 2 negative signs go away. G phi is 0, R phi is 0, S phi is G - R, generation - recombination rate. So, that is your continuity equation, you will recall. So, now the important thing is, we have shown it is derivable from the Boltzmann Transport Equation.

And we have shown how to derive it. We will call it as a carrier balance equation. Let us look at the next equation. Before that there are couple of comments regarding the recombination rate R here. Now please note this R is this R and it is not R suffix phi. R is the recombination electron-hole pair recombination whereas R phi is the loss of n phi because of momentum changes scattering.

So, we express the recombination electron-hole pair recombination rate as the carrier concentration - the equilibrium carrier concentration by minority carrier line. So, this is a form that we need to bear in mind. Now for instance in silicon minority carrier life time changes from nanoseconds to seconds that is the order. For comparison we have also given here the energy relaxation time and momentum relation times which will appear in the equations that we are going to consider shortly.

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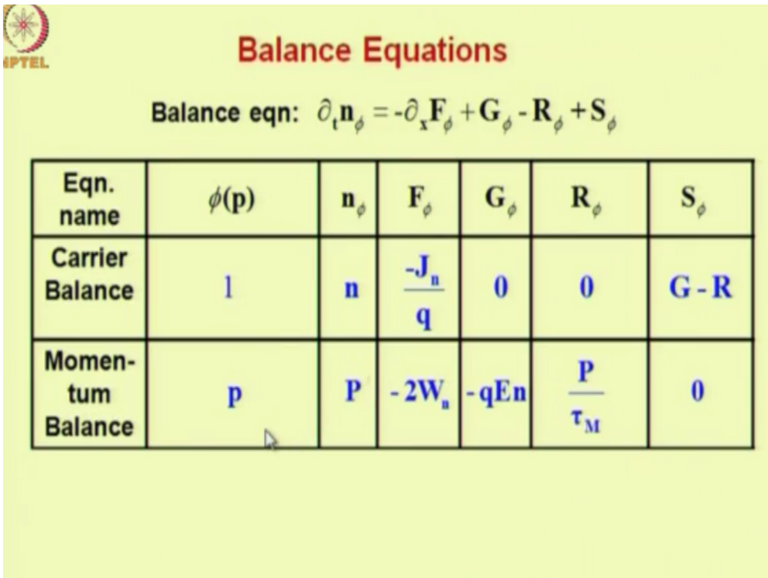

Let us look at the momentum balance equation you get that by choosing phi P = P because then n phi becomes the average momentum density capital P. Now please note that the symbol P is being used for multiple quantities. Now this one of the problems because in this course there are lot of quantities we are dealing with and so this kind of situation arise so small p or lower case p represents the momentum of a state.

It also represents whole carrier concentration, right? On the other hand, capital P will be used for average momentum density. So, small p is associate with an individual state, capital P is the property of an ensemble, okay. Now depending on the context you can decide whether P represents momentum or carrier concentration, right but capital P is momentum density of an ensemble. So n phi becomes average momentum.

Now that is very clear from this formula. So, if I choose phi i as Pi, when you multiply Pi/fi and sum you will get the average value of the momentum, right. So, that is what is shown here. On the other hand, F phi can be shown to be - 2 times the kinetic energy density. Let us look at that. Now fi is coming here. If I choose phi i as Pi we have chosen phi as P.

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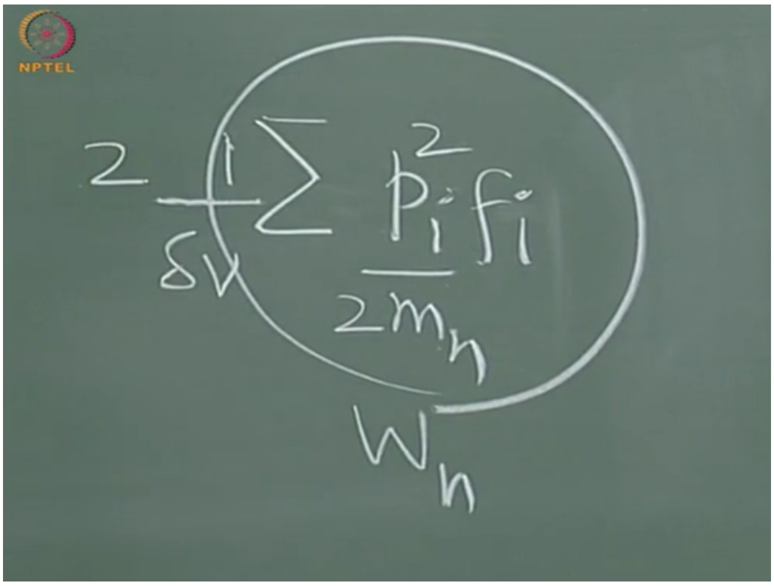

Now, that formula is Pi into fi into Vi. Let us look at this term. Vi, I can write as Pi/Mn. Thus this Pi and this Pi if I club and this is what I get. Now, if I divide by 2 and multiply by 2 this quantity is nothing but I divide by delta v also. This quantity is nothing but Wn, the average kinetic energy density because Pi square/2Mn is the kinetic energy of the electron having momentum Pi.

So, this is the average kinetic energy for the ensemble, okay. So, kinetic energy density and 2 is coming out because you are dividing here by 2. So, this quantity turns out to be 2 times Wn. So, the 2 times Wn term has been entered here. I just want to remark that there was a negative sign in the slide that I showed earlier that is not correct. So that has been corrected here it should be positive 2 times Wn.

Now let us look at the next term G phi. How do you get - q into E into n? So, G phi is this term here. We have to put phi = P. So, if you put phi = P dou phi/dou p becomes one. So, this goes out. So, you are simply left with sigma of fi divided by delta v. Now we have already said that this is nothing but the carrier concentration n and F is - q times E that is the force and therefore G phi becomes - qE into n.

So that is what we shown here. Let us look at the next term R phi. It is shown as the momentum density P/tau M. R phi is the term here. Now the n phi for us is the momentum density. This is momentum density under equilibrium. Now you know that under equilibrium the carriers have no net motion in any direction. Therefore, the momentum density of carriers in equilibrium is 0. So, this term is 0 and tau phi is the momentum relaxation time.

We have remarked earlier the tau phi is the time taken by the quantity n phi, in this case the momentum to relax to equilibrium when there is a scattering effect on the electrons. So, that time is momentum relation time and that is why you have this formula p/tau n, here. The term S phi is 0 because generation recombination processes do not contribute any momentum. So, this term S phi has been shown to be 0.

Now, often we are interested in the current density Jn rather than the momentum P, while momentum P is a physical quantity the quantity of practical interest which depends on the momentum directly is the current density. In device modeling we are interested in modeling the current density.

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Balance Equations

Balance eqn: $\partial_t n_\phi = -\partial_x F_\phi + G_\phi - R_\phi + S_\phi$

Eqn. name	$\phi(p)$	n_ϕ	F_ϕ	G_ϕ	R_ϕ	S_ϕ
Carrier Balance	1	n	$\frac{-J_n}{q}$	0	0	G - R
Momentum Balance	$\frac{-qp}{m_n}$	J_n	$\frac{-2qW_n}{m_n}$	$\frac{q^2En}{m_n}$	$\frac{J_n}{\tau_M}$	0

Now you can cast this equation of momentum density which is in terms of P in terms of Jn that is what we shown here. If you change the function phi P from P to - q/Mn into p. So, all that you are doing is you are multiplying the previous expression by - q/Mn. Then the momentum density P becomes Jn the kinetic energy density 2 times Wn becomes -2qWn/Mn.

The quantity -qE into n becomes q square En/Mn and the quantity momentum density/tau M becomes current density/tau M. Therefore, the momentum balance equation, the equation for Jn is often regarded as the momentum balance equation.

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Balance Equations

Balance eqn: $\partial_t n_\phi = -\partial_x F_\phi + G_\phi - R_\phi + S_\phi$

Eqn. name	$\phi(p)$	n_ϕ	F_ϕ	G_ϕ	R_ϕ	S_ϕ
Carrier Balance	1	n	$\frac{-J_n}{q}$	0	0	G - R
Momentum Balance	$\frac{-qp}{m_n}$	J_n	$\frac{-2qW_n}{m_n}$	$\frac{q^2En}{m_n}$	$\frac{J_n}{\tau_M}$	0
Energy Balance	$\frac{m_n v^2}{2} = \frac{p^2}{2m_n}$	W_n	F_W	EJ_n	$\frac{W_n - W_{n0}}{\tau_E}$	S_E

We will write that down. Dou Jn/dou t = 2q/Mn into dou Wn/dou x +the generation term that is q square En divided by Mn the recombination term -Jn/tau M. So, the generation recombination are not electron-hole pair generations or recombination's they are G phi and R phi, okay. The term corresponds to generation and recombination is 0, so we are not writing that down.

The term corresponding to electron-hole pair generation and recombination that is 0 that is why we are not writing it down. Now similarly, let us look at the energy balance equation. Now you might think why do we have to go in for energy balance equation. We are interested in the carrier concentration n and the current density Jn.

Now the reason why we need to consider the energy balance equation is because if you look at the equation that we just now wrote down, in the equation for Jn you have the kinetic energy density coming in. So, unless we solve for that we cannot get Jn. So, let us write down the terms in the energy balance equation. This is what we shown here. So, you get the energy balance equation by choosing phi P = P square/2Mn that is the kinetic energy.

Then the left hand side n phi becomes Wn, now that is very easy to see. Let us look at that. So, if you choose this phi as P square/2Mn you know that this quantity becomes Wn. We have written down this expression in the previous lecture. F phi, now we are not writing any expression for F phi we are just leaving it as the flux of kinetic energy and that is shown here with the simple F suffix W.

We will discuss shortly what we do with this term. Let us move on to the term G phi. This is written as E times Jn. So, let us see how do you get E times Jn. So, you take G phi expression dou phi and dou p.

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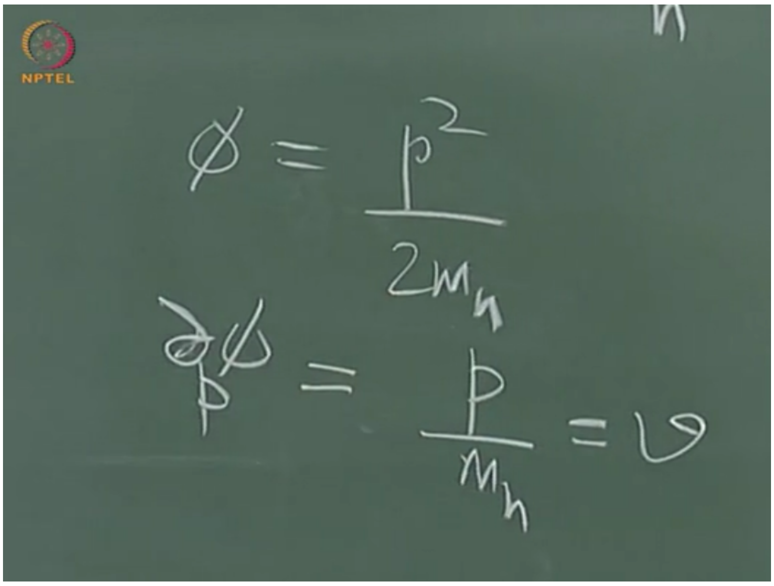

Now, if phi is P square/2Mn to differentiate with respect to P you get P/Mn. Now that is nothing but the velocity, right. So, either you can use V or P/Mn.

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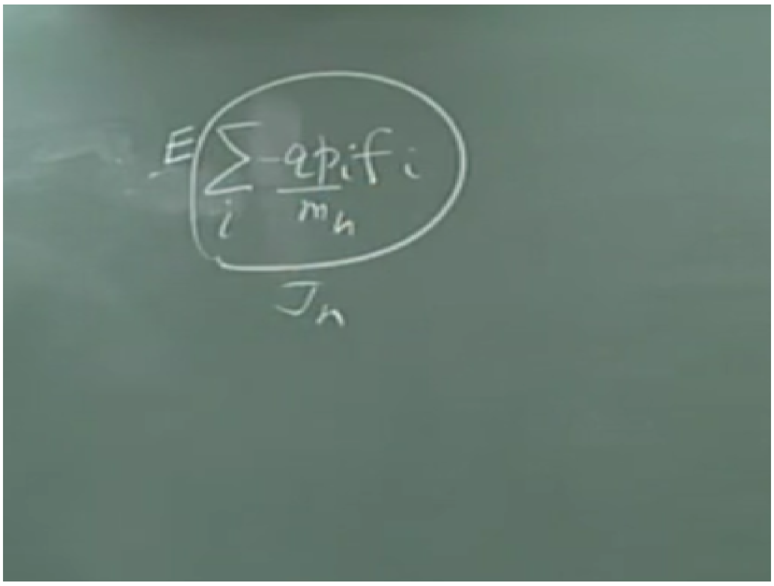

Now, here you have fi, so what you have here is fi into pi/Mn. This F is - q times E and we know let me push that q/Mn inside that - q times pi fi/Mn this nothing but the current density Jn. That is how you get E into Jn. That is the E into Jn term. Finally, or just before the final step R phi is written as Wn - Wn0/tau E. This is straight forward R phi is n phi - n phi 0/tau phi.

So, n phi is Wn the equilibrium value of Wn is Wn0 kinetic energy density under equilibrium and the time constant tau is the energy relation time because this time constant talks about how the energy relaxes to equilibrium value, right because of collisions, that is energy relaxation time. So that is how you get the term Wn - Wn0/tau E. The term S phi is retained here as S Suffix E because it is energy balance equation.

Just like the term, Fw has been retained as the flux. We will shortly discuss what do we with this term SE. Right now towards the close of the lecture let us write down that energy balance equation.

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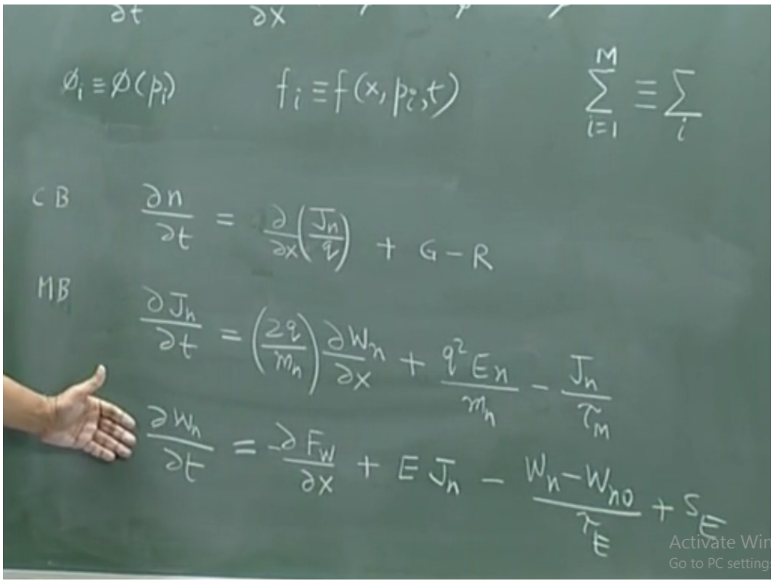

Dou Wn/dou t = - dou Fw/dou x +the generation of energy because of electric field that is E times Jn is nothing but the so called giving rise to heat - the recombination that is Wn Wn0/tau E so that is R phi and then S phi that is we simply we leave it as SE. So, now these are the equations. What do we do with Fw and Se? This we will discuss in the next lecture. For now, let us summarize the important points.

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So, in this lecture, we have developed the second approach of dealing with Boltzmann Transport Equation. The first approach was use the solution to the distribution function in particular use the Displaced-Maxwell Approximation and then derive n and Jn from this expression. Second approach that we discussed in this lecture, in today's lecture we avoided solving for F.

Because it is a function of 7 variables, instead we modified the Boltzmann Transport Equation into balance equations for quantities which are of direct interest to us namely the carrier concentration, the current density and so on and we derive these equations for carrier concentration current density, kinetic energy density and we call these equations as the balance equations.

In the next lecture, we will see how these equations can be applied to explain velocity saturation, velocity overshoot and all these phenomena.