Semiconductor Device Modelling and Simulation
Prof. Vivek Dixit
Department of Electronics and Electrical Communication Engineering
Indian Institute of Technology, Kharagpur

Lecture - 37
Semiclassical Transport (Continued)

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Hello, welcome to lecture number 37, so today we will discuss about the relaxation time approximation. Now we know that it is very difficult to solve the Boltzmann transport equation, so some assumptions have to be made so that we can solve the Boltzmann transport equation.

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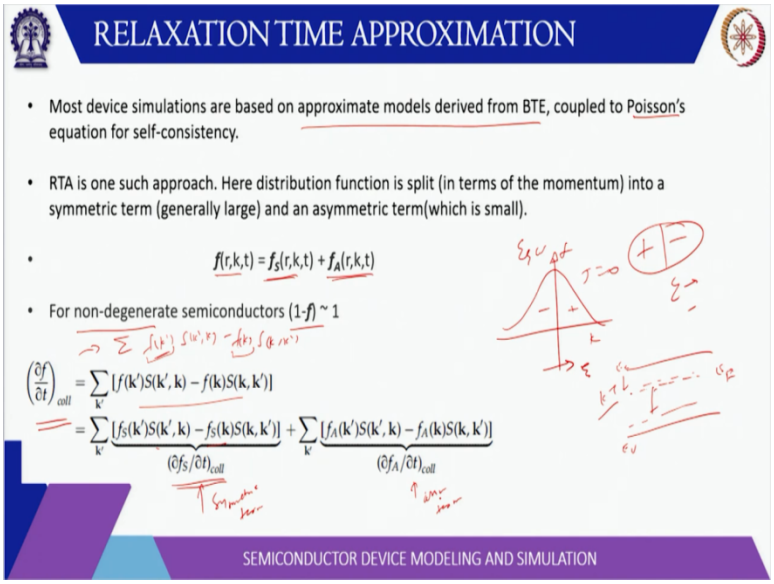

Now most device simulations models they are based on the approximate models derived from Boltzmann transport equation and then of course the driving force for these distribution function which is like electric field and all they come from the solution to Poisson equation because Poisson equation convert the charge distribution into the electric field. Now this electric field provides the impetus to change the momentum of the particles.

So, they have to be basically solved self consistently. Then relaxation time approximation is one such approach where we express this del f by del t in terms of single parameter which is called relaxation time. So, let us see how it is done? In general, what we can do your distribution function consists of several particles and we can divide this into two parts, a symmetric part and a symmetric part.

In equilibrium the distribution function has to be symmetric because there is no current flow. So, this plus and minus should balance so if you plot this f versus k then plus minus would balance out and then current should be zero, so it distribution function will be symmetric. Now when we apply certain electric field asymmetry will be created in the distribution function. So, we write this distribution function as sum of asymmetric which is equilibrium plus asymmetric distribution function.

Now additionally for non-degenerate semiconductor, non degenerate semiconductors are those where the fermi level lies inside the band gap and it is sufficiently away at least few k t from the bandage from either bandage. So, it will is within the E c - 3 k t or E v + 3 k t, so in this range this fermi level will be there. So, that means your 1 - f can be assumed close to one because this change in E f is not affecting the change in the concentration much here.

So, we can ignore. Then if we write this collision term del f by del t, so we can one versus f can be replaced as 1. So, overall, it can be done as this is del d by del t is sigma f is f s + f A so this is f of k prime times s of k prime, k - f of k times S of k, k prime. So, this f is basically f S + f A so if you write f as f S + f A then instead of this we will have two terms one in terms of f S other in terms of f A so, this is basically term in terms of f S so f S k prime - f S k and this expression **(()) (04:15)** is del f + by del t collision.

So, this effect of collision on symmetric term then for f A this is the effect of collision on asymmetric term. Now this asymmetry in the first place it came due to the applied field. Now if we consider different situations let us say at zero Kelvin at low temperature, at high temperature high field what will happen.

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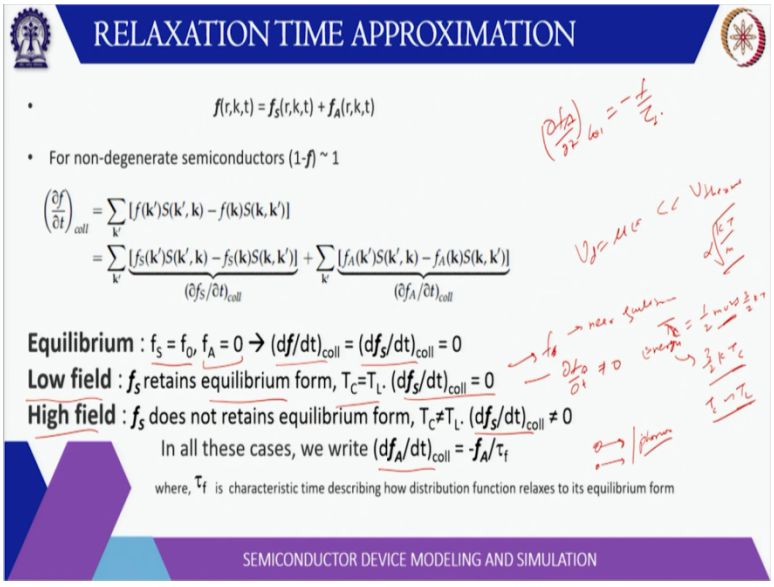

So, in equilibrium your f s is f 0 thus equivalent distribution function and this asymmetric term has to be 0 because it is equilibrium and then of course both del n by del t del f s by del t del f by

del t all will be 0. Now at low field f S is near equilibrium, so this is the assumption here that f S is near equilibrium or f is near equilibrium. So, that means the f S retains the equilibrium from that means your del f s by del t is 0.

And the velocity of these carriers inside the crystal are pretty small. Now there are two types of velocities you can see if you recall we said that drift velocity is Mu times electric field in case of semiconductor. Then we said under the assumption that this velocity is much smaller than the thermal velocity which was k t by m because energy is k t square root of k t by m. So, this is much smaller than the thermal velocity.

That means your temperature of the carrier which is we derived in previous while we discussed the distribution function half m v square + 3 by 2 k t that was energy. So, that is your energy and that can be written as three by 2 k t of the carrier so because this half m v square is quite a small. So, T c is same as lattice temperature, so in this case del f s by del t is 0 but del f by A by del t is non zero and in high field.

Now the velocity of caries is quite large so the carrier temperature is not equal to the lattice temperature. So, what happens when these electrons high energy electrons move through the crystal, they will transfer this energy to the crystal in terms of phonon. So, and till they lose their extra energy so in case of high field both del f s by del t the symmetric term and del f A by del t will be nonzero.

Now what we as you want the relaxation time approximation that in both the cases del f A by del t collision is given by – f A by tau where tau is a relaxation time. So, it is a characteristic of individual semiconductor.

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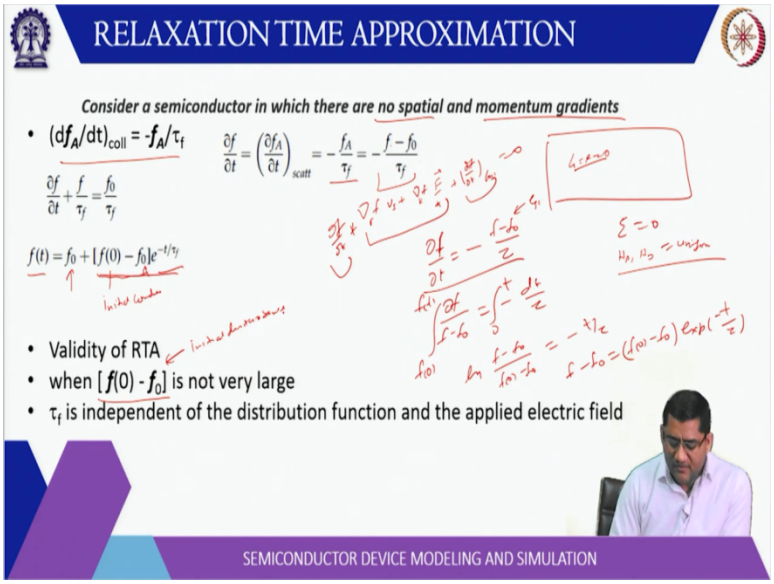

Now let us consider a semiconductor to understand what this characteristic time actually means. We are considering a very simple case where there is no special variation and there is no momentum gradient. So, that means if you piece are consider a piece of semiconductor there is no electric field so that means electric field is equal to 0 and there is no concentration gradient or doping gradient.

So, N A or N D are uniform or due to any other injection and all there is no there is no concentration gradient. That means only term that is there is the collision term, so if you write that Boltzmann transport equation then del f by del r times v g + del f by del k times f by h bar + del f by del t due to collisions and of course we are also assuming that generation G combination is also of 0 there is no net generation so that is terminal zero this is equal to 0.

So, what means can say that there is a delay by delta here so all three terms are there. So, now these two terms are zero so only term is remaining del f by del t + del f by del collision. So, they should be equal to 0, so del f by del t basically is - del f by del t collision. So, we can write del f by del t is simply - f A by D tau. Now what is f A? f - f 0. Now if you see at the sign here negative sign it means it is a rest restoring force.

So, del f by del t = - f - f 0 by tau, so where f 0 is the equilibrium distribution function. So, if it is deviating from equilibrium let us say f is more than f 0 then the gradient of f will become

negative so that it reduces the f. Let us say f become less than f 0 then the gradient becomes positive so that means it will try to increase the f. So, this collisions inside the semiconductor they their purpose is that they try to bring the equilibrium.

Then of course if you solve this equation del f by del t so you can write del f by f - f 0 s - d t by tau and then if you integrate it let us say initial let us say at equal to 0 is f 0 to some f at t and this is 0 to t. So, this will be log of f - f 0 divided by f 0 - f 0 will be - t by tau, so you can write f - f 0 will be f 0 - f 0 times exponential - t by tau. So, your f is basically f 0 plus this difference times e to the power - t by tau.

So, your f t is basically the equilibrium function plus initial condition minus the equilibrium distribution. So, if there is a division from the equilibrium distribution and that equilibrium distribution the deviation or delta f will decay exponentially with the time t f. So, that is a relaxation time and then of course this RTA will be valid when this f 0 means that initial disturbance it is initial disturbance is small enough.

Now S **(()) (11:48)** is it is much smaller than f 0 then of course this tau is independent of the distribution function and the electric field. So, that is also required to be able to define the relaxation time approximation.

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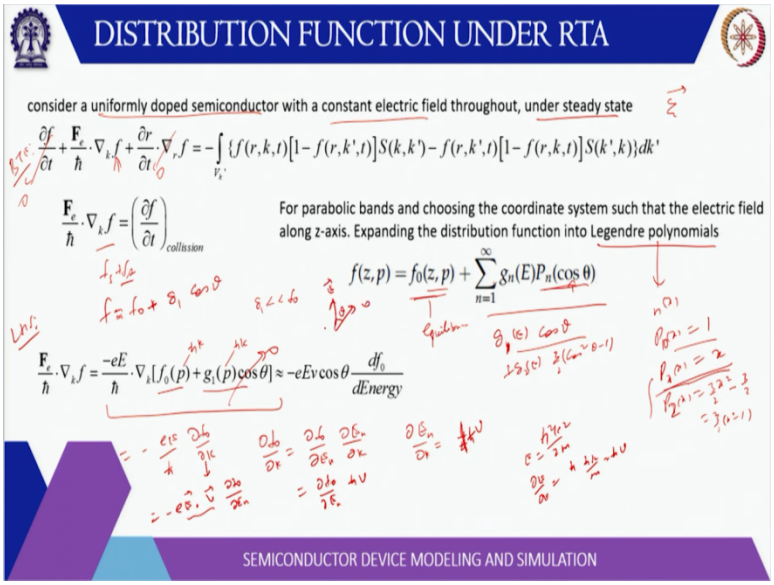

Now let us further consider this is your Boltzmann transport equation BTE and we are considering a uniformly doped semiconductor with a constant electric field. So, compared to the previous case now what we have done, we have introduced a electric field E. Now this electric field is uniform throughout the piece of semiconductor and this is under steady state. So, what will happen because this is a steady state so del f by del t has to be 0 and there is no concentration gradient.

So, this term will also be 0, so only term is applied force by h bar times del I by del k = del f by del t collision. So, you can write it here this f can be written as f symmetric + f asymmetric that we can also do here and f symmetric is basically because we are assuming with a small field here and this f 0 is the equilibrium distribution function. Then f asymmetric we can write in terms of legendary polynomials. So, why we are using the legendary polymers?

Because these are orthogonal functions so where these coefficients P n x, these are the legendary polymers, so this P 1 is basically 1, then P 2 is basically x and P 3 is basically x square times 3 by 2 minus half year. So, this is so 3 by 2 x square - 1, so of course we will consider only first two terms because we are assuming that the asymmetry or the disturbances is small. So, we can again write it as this is f 0 and this is term one onwards.

So, this will be g n times E, so g 1 E times P 1 cos theta, so this should be I think zero then this would be one this should be two so g 1 E times P n x so P 1 x will be x. So, this x is the cos theta here and this is the cos theta so g 1 cos theta + g 2 E times 3 by 2 cos square theta - 1 and where theta is basically a angle between the momentum and the electric field. So, let us say this angle between the momentum and electric field.

So, if the field is small, we can consider on the first term. So, what we can write? We can write f = f 0 + g 1 cosine theta so f can be approximate like this and then we substitute it here. So, to this f here so on the left side we get this expression - E which is of electric field times charge is the force so force by h bar times del k. Now p is h bar k here times cos theta. Now we are adding f 0 and g 1 and by definition this g 1 is much smaller than f 0.

So, when they come as addition you can ignore this part basically, as far as this equation is concerned the left-hand side. So, this is the left-hand side so what you have here - e E by h bar del k f 0 so you can write del f 0 by del k. Now generally we deal with the energy, so what we can write this del f 0 by del k can written as del f 0 by del e which is energy times del E by del k and daily by del k we know.

That del energy by del k is 1 over h bar times velocity because E if you assume the parabolic band so E is h bar square k square by 2 m that is h bar times v. And del E by del k will be h bar times h bar k by m that is h bar times v so del E by del k will be h bar times v, then we substitute here so this will be del f by del E times h bar v. Then this we substitute here, so what we will have here - e E electric field dot v times del f 0 by del energy.

And then e dot v is basically e v cos theta because we are assuming that electric field and the velocity, they are at angle theta. So, this is a general situation and we will cover for all the angles, so let us say now angle is let us say now is theta. So, this we have learned the left side. Now let us go to the right side which is the collision term, so here we have to integrate over k prime.

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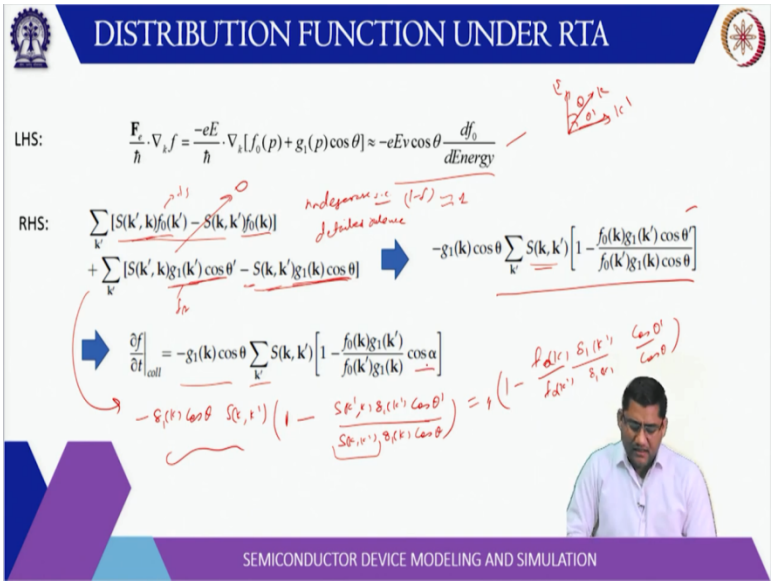

So, left side we have only drive this expression. Now on the right side we have this collision term, so probability of distribution from S k prime to k times f 0 into 1 - f 0 and of course we are

assuming a degenerate semiconductor non degenerate semiconductor. So, f 1 - f 0 is close to 1 so we can just write f 0 here and f 0 here and this is the f symmetric and this is f asymmetric term. Now if you recall the principle of detailed balance then we know that S k prime k by s k prime is the ratio of f 0 y f of k prime.

So, this first term actually goes to 0, so this first term actually equals to 0 using the principle of detailed balance. Now the remaining is g 1 k prime cos theta prime and g 1 k cos theta. So, what we can do? We can take g 1 k cost theta outside so - g 1 k cos theta take out, then you will have S k, k prime here and then this term you to divide by the second term. So, this will be let me simplify here - g 1 k times cos theta s k, k prime.

So, this we have taken outside so this is become one then - S k prime, k g 1k prime cos theta prime divided by S k, k prime g 1 k times cos theta. So, what we have assumed here that let us say electric heat is in this direction so this was a theta here for k. Now it has this has scattered to some another angle let us say theta prime this is the k prime so, this is what we have assumed here.

Now this theta prime will determine the k prime, then we have to integrate over this theta prime. So, that will give you that overall right hand side. Now if you recall the principle of detailed balance then S k prime k by S k prime will be 1 - so this become as it is times S k prime case if you look at the first string so it is f 0 k. So, this is f 0 k by f 0 k prime then g 1 k prime by g 1 k times cos theta prime by cos theta.

So, this is what we have got here basically, so if you use right hand side and the left hand side then we can write from this we can calculate this del f by del energy and in terms of g 1 k. So, the right side is basically - g 1 k cos theta summation over k prime as k prime into 1 - f 0 k g 1 k prime by f 0 k g 1 k cos alpha.

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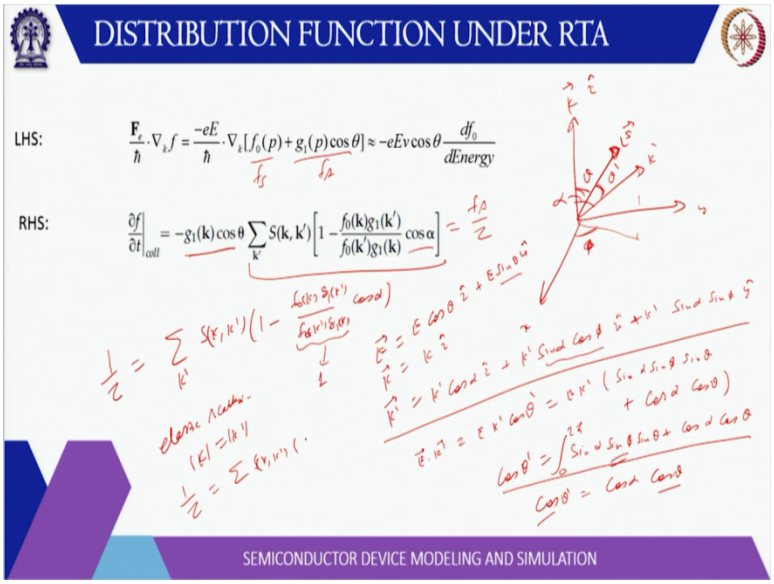

So, how do we get this cos alpha? Let us look here let us say your k is somewhere in this direction then this is your electric field let us say this is z direction and this angle is theta. Now this k prime is scattered to another angle which theta prime to this electric field and then this is your y axis this is your x axis. So, let us assume by the without the loss of general d that is E vector is in y z plane.

So, your E can be written as magnitude E cos theta in z cap + E sin theta in y cap and of course your k vector is 0 in x cap. So, it is basically k in z cap direction and the k prime vector is angle theta prime it is scattered at theta prime and let us say this angle is with respect to case this angle is this alpha. So, with respect to case it is alpha. Now theta prime is the angle between electric field and the k prime.

So, let us say this is not in same y z axis this is angle this makes some angle phi in the x y plane so all the three component can written as z component is of course k prime cosine alpha is z component + k prime sin alpha cos phi is x component + k prime sin alpha sin phi is y prime. Now from this we can take this e dot k prime will be e times k prime the angle between them is cos theta and from these vectors we can multiply x component y component.

So, this will be E k prime then x component here is sin alpha cos phi and this is 0 here, so y component sin alpha sin phi times sin theta + z component is cos alpha times cos theta. So, from

this we can find out this is cos, so cos theta prime is equal to sin alpha sin phi sin theta + cos alpha cos theta. Now this is true for arbitrary theta prime and then we when we average it for all the theta primes when we average it so this is theta and theta prime.

So, this phi basically can vary you know theta is the initial angle between the electric field and the wave vector theta prime is the final angle between the electric field and the wave vector and alpha is a scattering, angle between k and k prime and phi is along the angle with respect to x axis in x y plane. So, this is basically spherical coordinate, so if you average it over phi 0 to 2 pi this will go system will go to 0.

So, your cos theta prime is cos alpha times cos theta so the ratio of cos theta prime by cos theta can be replaced by cos alpha, so this is what we have done. So, this ratio cos theta prime by cos theta is replaced by cos alpha here where alpha is the angle between two wave vectors k and k prime. Now this you can replace you can write in terms of f A by tau. Now f A is what g 1 k cos theta this is f A asymmetric term.

So, this is f S symmetric term this is f A, so this you can write from here that 1 over tau is sigma S k, k prime these are the scattering rate times 1 - f 0 k g 1 k prime y f 0 k prime times g 1 k cosine alpha and this average over k prime. So, this is the overall scattering rate. Now we can consider a scenario, let us say this is elastic scattering in elastic scattering k = k prime. So, that means f 0 k by f 0 k prime g 1 k by g 1 k prime will be 1.

So, your for elastic the tau will be sigma S k, k prime times 1 - cosine alpha so that is one special case.

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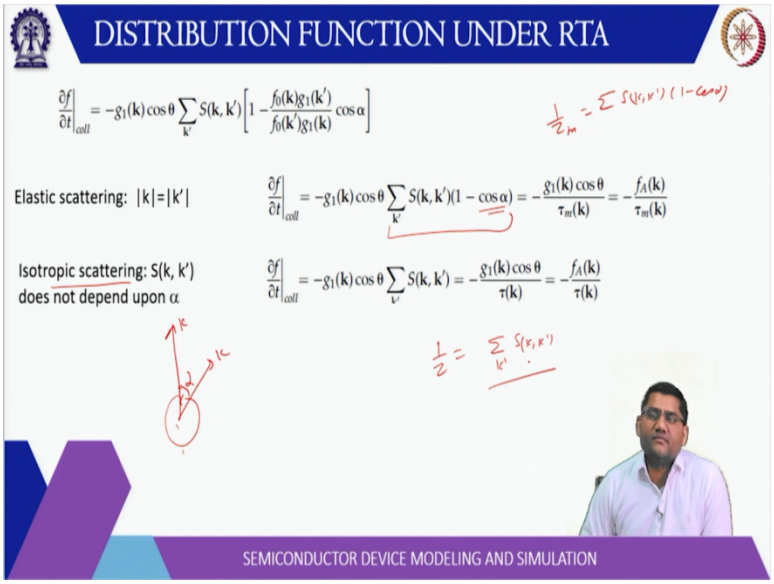

So, you can write it as this will be your tau, so tau m is 1 over tau m is sigma S k, k prime times 1 - cosine alpha. Now if there is isotropic scattering, isotropic scatter means this is your k and then this is your k prime, this alpha can be anything. So, this will cover all the equal probability it will equal probability of having angle 0 to pi and so on. So, that means if you add them all of them this term will go to 0, so in this case one over tau will be sigma S k, k prime.

So, the tau in case of isotropic scattering is just summation of S k, k prime, so we will do some for this s for all the k prime.

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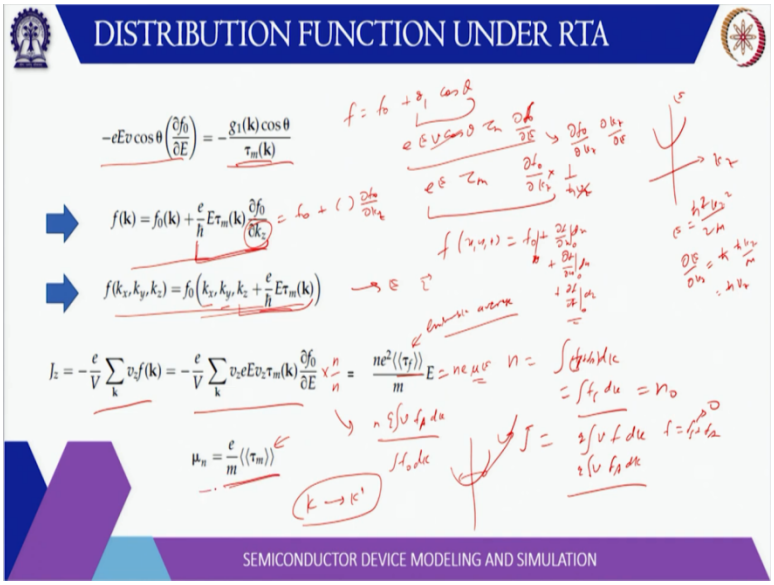

Now if you create the left-hand side equal to right hand side, so what we have done here for either case we are writing this some tau effective some name is given. So, let us that is tau m here, then from this we rearrange it because your f is f 0 + g 1 cos theta, so g 1 cos theta can be done from here the g 1 cos theta is e E v times cos theta and tau m times del f 0 by del E and now this is del f 0 by del E, this x was del f by del k.

So, del f by del E can be written as del f by del k z times del k z by del E. Now this is EK diagram in z axis, so this is k z this is E k, so E = h bar square k z square by 2 n this is E so del E by del k z S h bar h bar k z by m that is v z. So, h bar times V z so del E by del k z is h bar v z so del f by del e can be done S del f phi del k z times del k l by del is 1 over h bar V z. Now V z is basically v times cos theta because initially we assume that electric field is in the z direction.

So, this V cos theta and V z will cancel out, so what you will have e E tau m times del f by del k so e E tau m by del t by del k. Now if you look at this expression carefully that ah the distribution function is f 0 + some term times del f 0 by del k z. So, if you compare this thing with the Taylor expansion because we know that for Taylor expansion as it is x y z is can be written as f 0 + del f by del x times dx + del f by del by dy + del f by del z dz.

And this is at this r 0 position where x 0 y 0 z 0. So, this is at x 0 y 0 z 0, so this is basically the change in dk z. So, this will basically add to the k z part so your equilibrium function is now distribution function is now k x k by and k z plus this term e by h bar E tau by E tau k. So, this is your overall distribution function when you apply a electric field in z direction, so your distribution function modifies like this.

So, for a very simple case we can directly solve the distribution function once we know the distribution function we can integrate and find the different moments. Of course, n will not change because n is integral f dk so that is f symmetric + f asymmetric, f asymmetric is very small. So, it will be simply f s times dk and that we have already derived when we discuss the distribution function.

So, this will be same as n 0 so this will not change the carrier concentration. Now the electric current is q times v times f dk, so this is done here as summation and of course sum over k here f is f symmetric + f asymmetric due to symmetric this will be 0 because this is symmetric and + k - k will cancel out. So, you will simply have q times v times f asymmetric dk so that will be there, so this is what done here.

Now if you see here if you multiply this thing by n divided by n so n is basically integral f dk, so this can be written as q times v times f a dk times n divided by integral f 0 dk and this is f asymmetric dk. So, you will have if tau is constant then n e square tau by m will come otherwise, we can replace this tau by the average value of the tau. So, this is called n symbol average and that is basically the time that is important for us.

And then of course if you compare this thing j = n e mu E. So, if you compare you get the expression for mu from this 1 so mu = e tau by m. Now this tau is not just the actual time between the collisions but it is the average value of that relaxation time because the this is scattering from k to k prime will depend you know because if you are scared there are multiple valleys are there.

So, this electron may be scaling from one valley to another valley that is called intra valley scattering that is a electron may distribute this electron may is scattered to the same valley. So, each scattering process will have different time constant or there may be variation. So, it is basically the average of this tau of weighted average, so this we say weighted average. So, its average skating time times e by m is the mobility.

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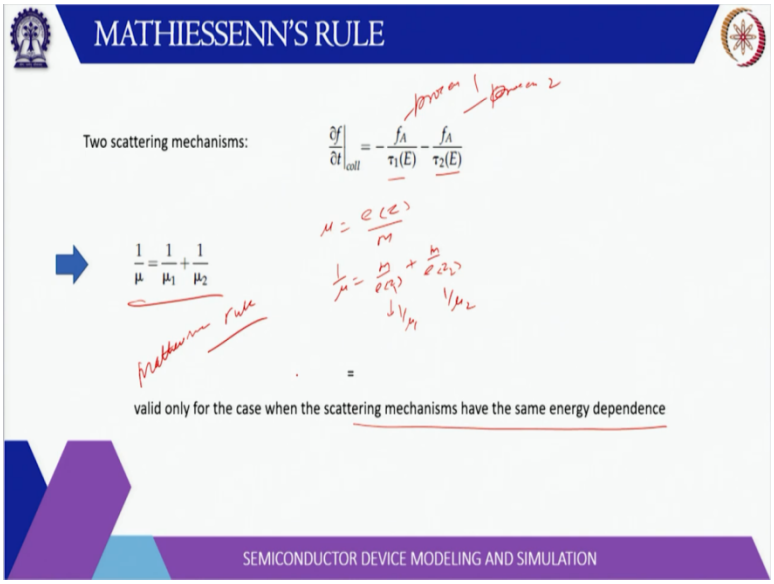

And if there are two processes so there is a process 1 and there is another process 2. So, what will happen del n by del tool will be f A by tau 1 + f A by tau 2. So, these are two skating mechanism and of course when we try mu so mu is e average tau by m. So, now 1 by tau is a scattering rate, so these scattering rate are adding up. So, what will happen 1 over mu which is m by e tau they will add up.

So, 1 by mu will be due to is this process one plus m by e tau this is tau 1 tau 2. So, we can write this is 1 by mu 1 this will be 1 by mu 2, so overall mobility is the weighted average. So, 1 by mu is 1 by mu 1 + 1 by mu 1 and this rule is called Matthiessen rule. So, there may be n number of processes and the only condition is that it is valid for only for those cases where scattering mechanism of same energy dependence so if the energy dependence is different.

Now how the energy dependence comes to the picture? You are integrating here. So, this tau m may have some energy dependence and that energy dependence is different for different mechanism, then we cannot use this Matthiessen rule. But we use it you know in most of the semiconductor modelling and that may be valid for low field scenario but there is a strict criteria for using this Matthiessen rule.

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So, in this lecture we have discussed this, so in this lecture we have discussed the relaxation time approximation and we have solved for distribution function under very restrictive scenario. Thank you very much.