Semiconductor Device Modelling and Simulation
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Lecture-53
Problem Session-8

Hello, welcome to lecture number 53.

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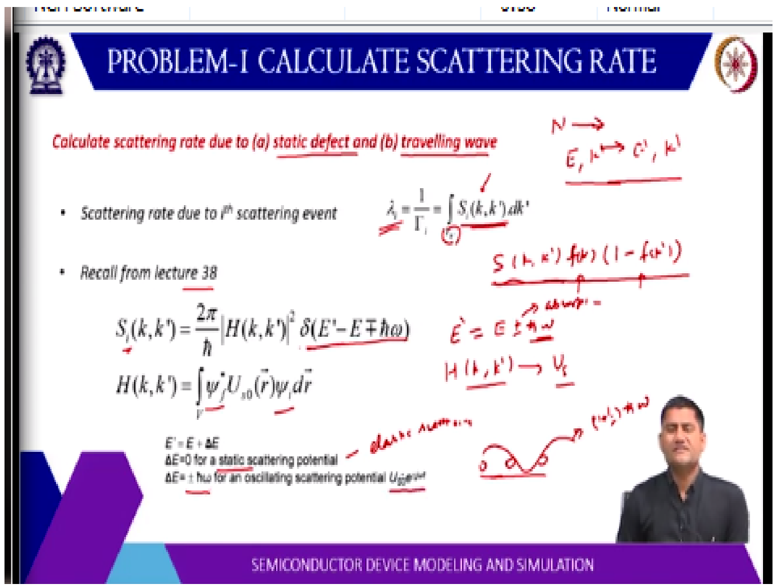

In last class we discussed about the Monte Carlo simulation, now we will take up some problem related to Monte Carlo simulation. In Monte Carlo simulation we discussed that we started with n number of particles and we track them basically through certain scattering event. Energy E and the wave vector k, when it is scattered it has new energy E prime and wave vector k prime and then of course we track these particles and from their tracking we estimated what is there over all response to particular excitation.

Now as a first problem let us take or calculate the scattering rate due to defects. We will consider 2 defects here; one is static defect another defect which is traveling wave type. So, your static defect can be the ionized impurity scattering, traveling wave defect can be your phonon, acoustic phonon or optical phonon. Now let us recall this S k comma k prime is the scattering probability. And then we say the scattering rate from k to k prime is basically scattering probability multiplied the probability of finding electron in k and then probability that there is a empty state in k prime, so that is 1 - f of k prime.

And then of course we estimate that if we say this is basically full, this is empty you can just say S of k comma k prime. So, let us assume this is S of k comma k prime then if we integrate it over all the k primes, we will get the overall scattering rate for is state wave vector k. Now if you recall from lecture number 38, we discussed that a scattering probability S comma k comma k prime due to ith scattering event is given by 2 pi by h bar h of k comma k prime square times delta E prime - E - + h bar omega.

This delta term here basically represents the conservation of energy, so that means your E prime is final energy and which should be equal to E the initial energy + - h bar omega. Here plus term indicate that there is absorption of some energetic particle with energy h bar omega and minus means there is a emission of this particle. So, these particles are actually low energy like phonons and they have low energies.

So, change in energy of the electron is quite a small, so this delta term basically represents the energy conservation. Then 2 pi by h bar, h bar is the reduced Planck constant, so it is a constant term here. H comma k comma k bar, k comma k prime is a matrix element due to the scattering potential let us call it U s. So, some scattering potential due to the defect or phonon may be there, so this is a matrix element due to scattering potential and then it is calculated as the wave function of the final state.

So, that is basically corresponding with the k prime times scattering potential times the wave function of the initial state and integrated over space. Another thing if you can note here for static scattering potential such as ionized impurity scattering, this change in energy 0. So, this is basically you can say it is an elastic scattering. For phonon scattering, so phonon basically involves the oscillation of these ions is basically, so due to this phonon scattering this is basically some kind of traveling wave is there, some kind of oscillation is there.

And these oscillations are quantized and their energy is given by some n + half h bar omega, where omega is the angular frequency of these phonons. So, the energy which is absorbed or released due to phonon scattering will be + - h bar omega. And their scattering potential will be represented by some function with e to the power + - g omega t.

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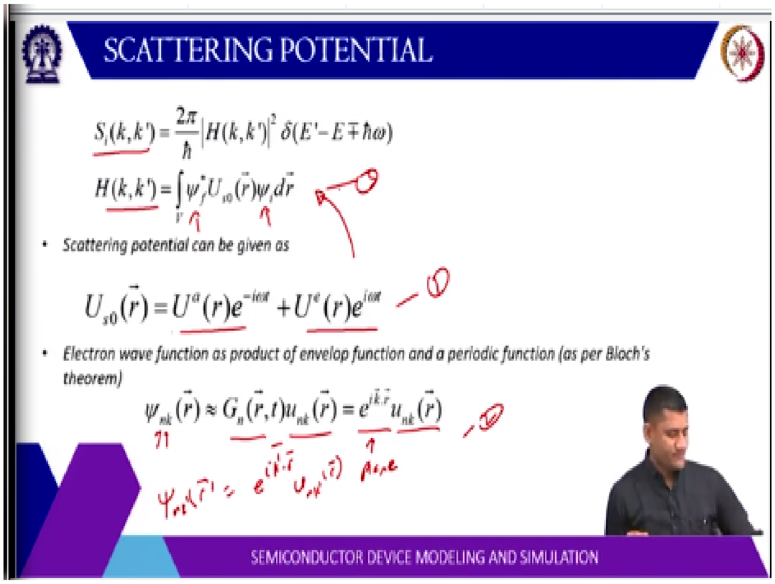

Now we have defined the scattering rate probability S i, then this matrix element H k comma k prime. Then scattering potential in general can be written as 2 components the absorbing condition or absorbing scattering potential and the scattering potential related to the emitting of these phonons. And when you substitute this scattering potential to calculate matrix element H, you have to substitute this wave function also initial and final state wave function.

And wave function for a nth state and wave vector k is given as a product of periodic function U nk r which is periodic in space and the periodicity of this function is same as the periodicity of the crystal multiplied by a plane wave. And so this can written as e to the power Iota k dot r which is equation of plane wave times this periodic potential U nk r, so this is psi nk. Similarly you can write psi nk prime will be e to the power Iota k prime dot r times U nk prime r. And then when you substitute 1 and 2 into 3rd equation.

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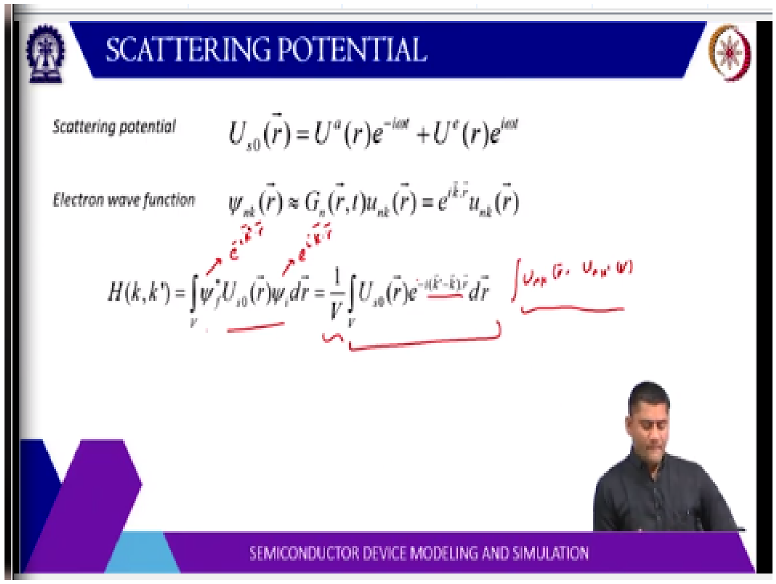

So, this is substituted here, now this term U nk r times U nk prime r, this will give rise to this raise to normalized condition here and overall integral can be written as scattering potential U s times e to the power Iota k prime k - k prime r dr. So, this is basically because this is a complex conjugate, so it will come e to the power -Iota k prime dot r and this will be e to the power Iota k dot r. So, if you take them together it will be e to the power Iota -k prime -k r, so this k prime is minus here and k as plus so minus, minus, plus.

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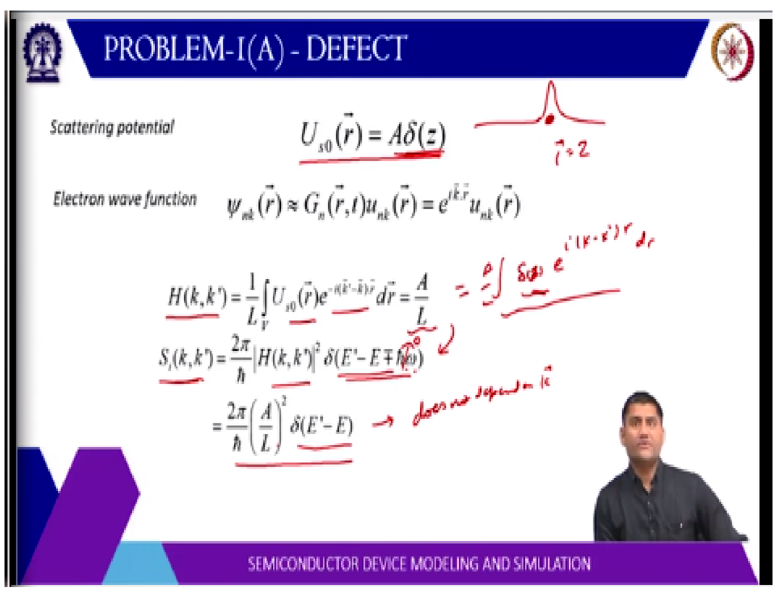

Now let us consider scattering potential due to a defect. Now defect as a nature, it is localized at particular position r = z, some position. So, you can say let us say it is some x = 0, y = 0 and z =

z at some position, so it is localized. So, it is scattering potential can be approximated by some kind of delta function basically. So, in the vicinity of the defect let us say it is influence is negligible and when it is at this defect it is basically very high potential basically.

So, you can say this A delta z, then when you substitute this A delta z to calculate the matrix element H of k comma k prime, so this will be U s 0 times e to the power Iota k - k prime r. So, this is basically A can be taken out and this 1 by v (()) (09:27) because this is we are assuming 1 dimensional, so 1 by v will become 1 by L, so this is A by L times delta z times e to the power Iota k - k prime r dr or you can say r z times dz that also can be done.

Now if you look at this function this is basically kind of Fourier transform for delta z function. And Fourier transform of delta is basically 1, so it will be simply 1 basically, so you will have simply A by L. Then of course when you substitute this matrix element to calculate the scattering probability for scattering from k to k prime there is 2 pi by h bar matrix element square times delta.

Now in this case there is no traveling wave, so no h bar omega, so this **is** basically term is 0, so it is simply E - E prime. So, this is basically means energy is conserved and there is no change in the energy and the scattering is elastic. So, this scattering probability S i will be 2 pi by h bar A by L square times delta E prime - E. And here you notice one more thing it does not depend on k or k prime. So, it is basically constant regardless of the wave vector.

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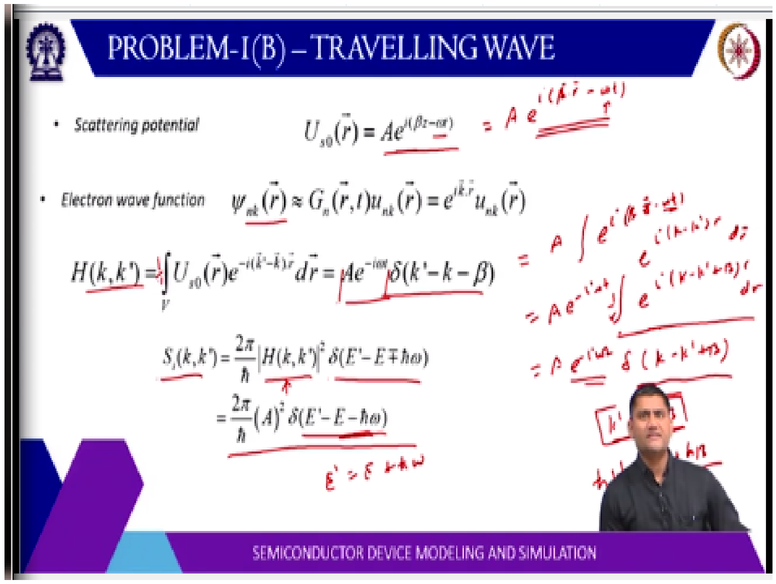

Similarly we can calculate the scattering probability due to traveling wave type of defects such as phonons. So, here we can represent the potential by e to the power Iota B z - omega t. And in general form it is basically A times e to the power Iota then beta dot r - omega t. Now this omega is basically the angular frequency of scattering potential and beta is basically some kind of propagation constant.

Now again if you substitute these electron wave functions to calculate this matrix element H of k comma k prime. Here you will get A can be taken out and this is e to the power Iota beta z - omega t times e to the power Iota k - k prime r dr. So, all these Iotas can be basically combined and omega t can be taken out because we are integrating with respect to position. So, A e to the power - Iota omega t can be taken out and in the integral we have e to the power Iota k - k prime + beta.

Let us write this also as as r. So, that is let us use this general expression A this is r times dr. Now integral of this exponential function is basically is a delta function basically. Of course there is a 1 by v is also, there is a 1 by volume is also there, so delta function. So, that means your A times e to the power -Iota omega t times delta of k - k prime + beta. So, if you compare here that means k prime = k + beta.

So, there is a conservation of momentum basically because the momentum is h bar k, so h bar k prime = h bar k + h bar beta. And because this k has changed and it is a e to the power -omega t also, so there will be change in energy also. So, when you substitute this matrix element to calculate the probability of scattering, so 2 pi by h bar matrix element square times delta E - E prime - E - + h bar omega.

And this is basically the magnitude of matrix element here, so the matrix element this magnitude will be simply A. Because e to the power -omega t magnitude is 1 basically, so it will be 2 pi h bar times A square times delta and this is basically the conservation of energy. And it says that E prime = E + h bar omega because there is a minus sign here, so this is -h bar omega is coming here. So, that way we can calculate for a given scattering potential or given a scattering type, we can calculate these scattering probabilities.

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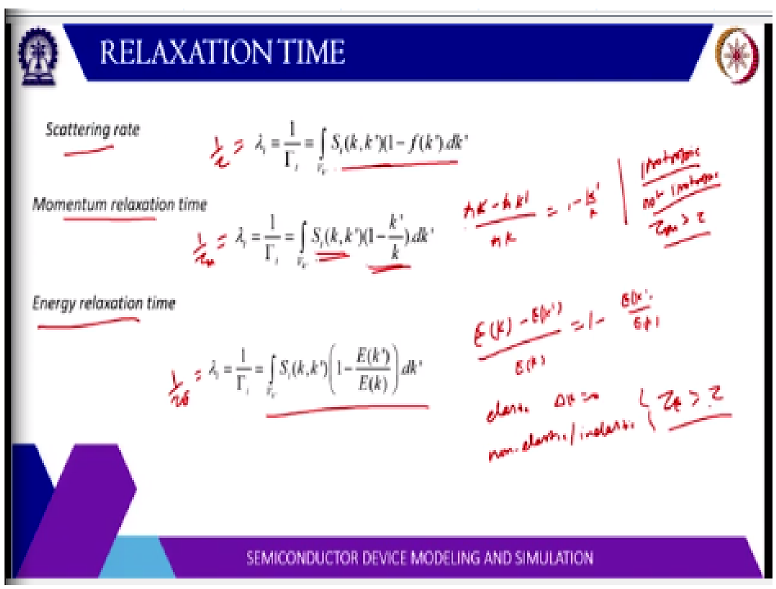

And once we have this scattering probabilities we can find out what is the scattering rate. So, that is basically integral S dk of course into f into 1 - f of k prime all those can be included. And then if you want to calculate the momentum reduction rate then this scatting probability can be multiplied with the change in momentum. Now change in momentum is h bar k - h bar k prime divided by h bar k.

So, h bar will cancel out and you will have basically 1 - k prime by k, so this factor is coming here, so that will be the momentum relaxation rate. Similarly energy relaxation rate, so it will be E k - E k prime the change in energy delta E divided by E k, so then of course you can write it as 1 - E k prime by E k, so you can calculate the energy relaxation rate. Now generally this relaxation rates are different from the scattering rates because not all the scattering events are causing the change in energy or causing the change in momentum.

There are some scattering which are isotropic, so they are basically altering the momentum to the maximum they are contributing to the momentum relaxation rate and which are not isotropic. Their contribution to the change in moment of relaxation it is small, so this is basically momentum relaxation time. So, this will be you can write test 1 by tau let us call it m, this we call it 1 over tau E and let us call it 1 over tau.

So, tau m will be more than tau as far as energy relaxation time is concerned there are some scattering which are elastic. So, for them this delta E is 0, there are some which are non elastic or inelastic, for them there is a change in energy. So, that means this tau E will also be more than tau. So, these are the different relaxation times that can be calculated from the calculated value of this scattering probabilities.

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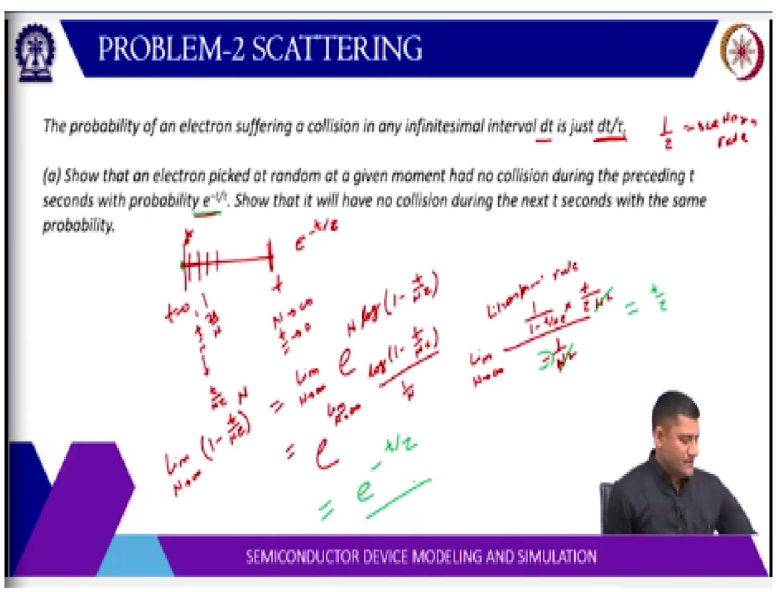

Now let us consider another problem with whose result actually we used in discussing Monte Carlo simulation. Let us consider that the probability of an electrons suffering the collision in any infinitesimal interval dt is just dt by tau, where 1 by tau is the scattering rate or you can say scattering probability. So, within dt by dt time the scattering probability is dt by tau. Now we have to show that electron picked up at random at a given moment had no collision during the preceding t seconds with probability e to the power -t by tau.

That means if you start at t = 0 or at t = 0 then you go till time t. Then in this period what is the probability that a particular electron does not have a collision? And that probability is e to the power -t by tau that we have to prove. So, we know that scattering rate is 1 by tau and scattering probability is 1 by tau and in time duration dt scattering probability is dt by tau, so what we can do?

We can break this region 0 to 2 into n number of parts, so we can consider very small parts basically. And that let us call it dt there are n number of part, so from t = 0 next is t by n, the next is 2t by n and so on. So, during this small period t by n probability of a scattering is dt by tau, so the probability of a scattering is dt is t by N divided by tau. And probability of not scattering is 1 - t by n that is dt by tau.

Similarly in the next interval which is also t by n because from t by n to 2t by n, so same probability is there for next cycle, for third interval, fourth interval and so on. So, that means for n intervals this probability will be 1 - t by n tau to the power n. So, that is a probability that electron did not have a collision from 0 to t, now what we have to do? We can assume that this N goes to infinity or that means this t by n goes to 0, so we have to evaluate this from limit N tending to infinity and what will be this?

We can write this one in the form limit N tending to infinity 1 - t by n tau to the power n. So, it can be written as exponential N log of 1 - t by N tau because e to the power log is basically same number. And by using the properties of this limit we can write this is e to the power limit N tending to infinity log of 1 - t by n tau divided by this n can written as 1 by n here. Now we have some numerator by denominator and if you recall there is a L hospital rule.

You can take the derivative of numerator and denominator, so if you take the derivative, so this denominator derivative is 1 by n square because d by dn of 1 by n is N to the power -1, so -1 into N to the power -2, so it is -1 by N square. And this log term is 1 over 1 - t by N tau multiplied by log x is 1 by x and this is 1 - c, so derivative 1 is 0 and this will be t over tau times N square. And then if you put limit N tending to infinity, so this is 1 by N square 1 by N square these 2 will basically cancel, that is different colours, this N square, this N square will cancel.

And this N goes to infinity, t is finite, so this will be 0 basically, so this will be simply t by tau and with a minus sign, this is a minus sign here. So, it can written as e to the power -t by tau and that is what we have to prove. So, that means for the time 0 to t the probability that electron will not have collision is e to the power -t by tau. And that is the reason we chose this exponential function while discussing the Monte Carlo simulation. So, we approximated this thing with exponential function.

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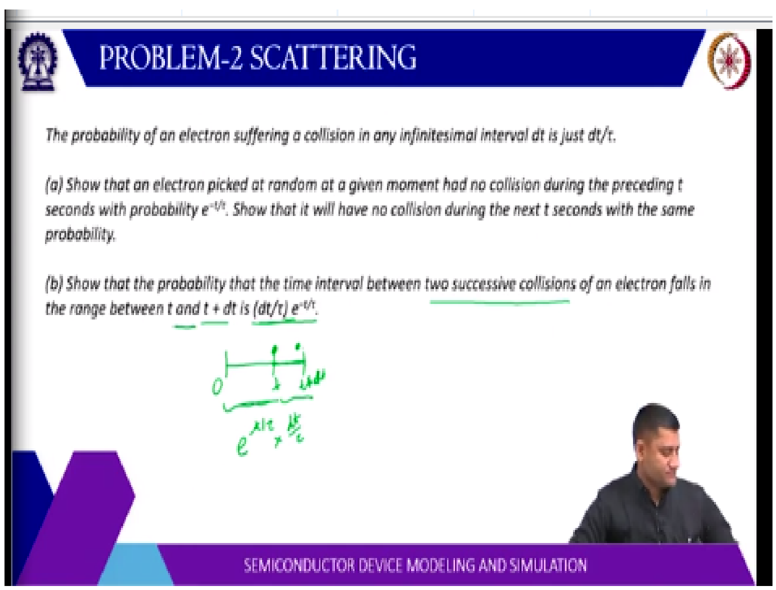

Now, so that the probability that the time interval between 2 successive collisions of an electron falls in the range between t and t + dt is dt by tau times e to the power -t by tau. So, that means you start with t = 0 and consider up to t until time t there is no collision. So, there is a first collision here at t = t, then second collision is between t + dt, so there is another collision in between these 2 regions.

So, what is the probability? That there is no collisions up to t that is e to the power -t by tau, so this is a probability of first collision at time t. Now between this time interval dt, there is another collision. So, this first collision at t which is e to the power -t by tau, so there are 2 successive collisions. So, first collision probability is e to the power -t by tau, so that means there is no collision till t, there is a collision at t, so that is e to the power -t by tau.

Then there is another collision if you start at t, so between t and dt there is another collision and it is probability is dt by tau. So, overall probability is basically the product of these 2 probabilities and that is what is shown here through the b part. So, this result also we used in discussing the Monte Carlo simulation.

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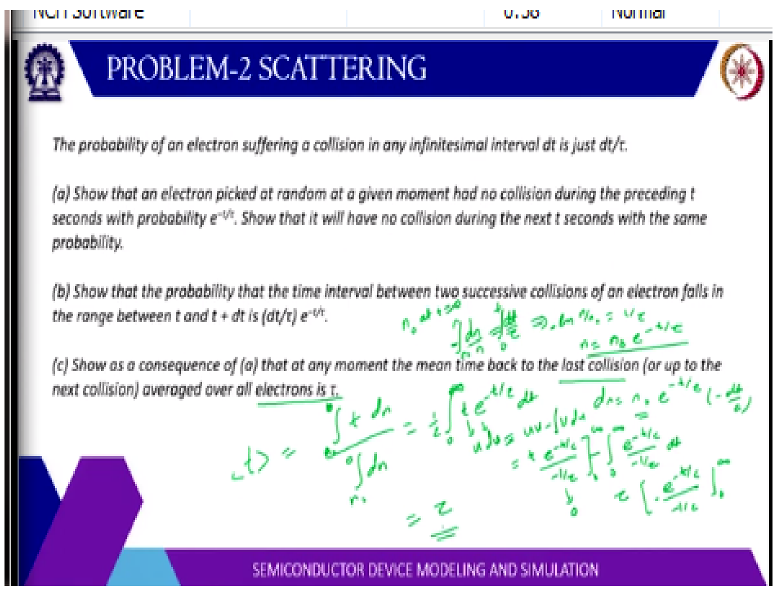

Then as a consequence of a that at any moment the mean time back to the last collision or up to the next collision averaged over all electron is tau, that you have to prove. So, this average time can be calculated as integral t dn divided by integral dn, so this t is the time for a collision. Then we can use this expression for N we know that the probability of collision is dt by tau, that is the probability of collision.

So, that means this is the probability of change in the number of electrons which have gone through the collision. So, you can write this as dn by n, so number of electrons that have collided but this is basically if there are n naught electrons at t = 0, let us say there are n naught electron at t = 0 which I have not gone through the collision. So, at next time this number will decrease basically.

So, let us say delta n or dn have gone through the collision, so now electron which I have not gone through the collision will be n - delta n. So, this dt by tau will basically change the ion, so you can write -dn by n is dt by tau. And if you use this one, so if you integrate let us say from n 0 to n and this is let us say 0 to t, so you will get log of n by n naught minus sign = t by tau and from this you can write n = n naught exponential -t by tau.

So, this is the relationship how the electron which have not gone through the collision changes with time. So, from this you can write dn = n naught e to the power -t by tau times -dt by tau and that you can substitute here, times t and it can be integrated. So, this dn let us say n naught to 0, this is 0 to some time t, this also has a dn, so you can write n naught to 0 here basically. So, when you integrate it this will be n naught here.

So, this n naught and this naught can be taken out, so this will in terms of dt, so what you will have here t times e to the power -t by tau then dt. And tau can be taken out and n naught will cancel out, so this will be 1 over tau and this is 0 to certain limit to infinity basically. Because at infinite time none of the electron is remaining which has not gone through the collision, so that means all the electrons have gone through the collision.

So, this can be integrated using integrations by parts, so if you recall that there is integral U dv it can be written as U v - integral v du. So, this is let us say u and this is v, so this can be written as u is t and integral this thing will be e to the power -t by tau divided by -1 by tau. And this is -du is 1 and dv is e to the power -t by tau divided by -1 by tau times dt and this is the limit 0 to infinity, this is limit 0 to infinity.

So, at t = 0 this is multiplied by t, so this will be 0 as infinite e to the power –t by tau, so this will basically be 0. And this will be tau can be taken out, so this will be tau and the integral e to the power -t by tau will be -1 by tau, so minus sign here 0 to infinity. So, at infinity this is 0, at 0 this is 1 by tau, so it becomes basically tau square, so tau square by tau will be tau. So, that has basically proves that time back to the last collision averaged over all electron is actually tau.

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So, that is all for today. So, in this lecture we have discussed problem related to scattering rate and the calculation of probabilities. In next session we will begin our discussion about quantum transport, thank you very much.