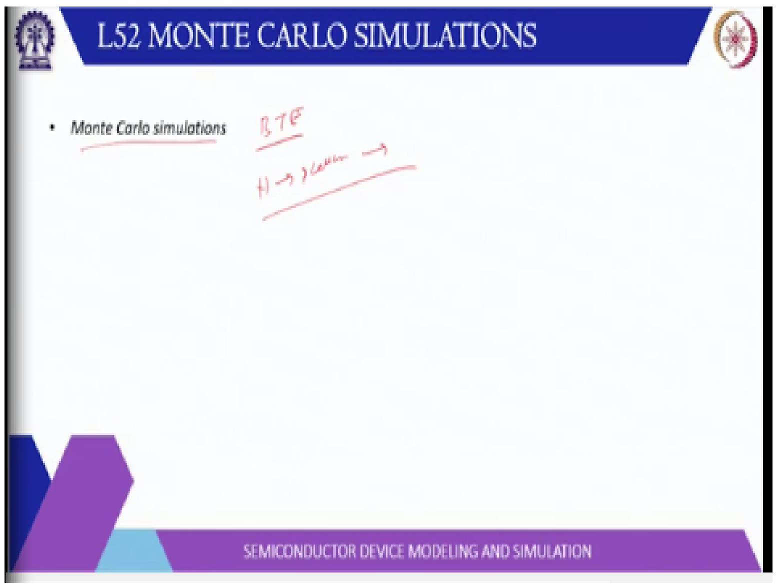
**Semiconductor Device Modelling and Simulation**
**Prof. Vivek Dixit**
**Department of Electronics and Electrical Communication Engineering**
**Indian Institute of Technology-Kharagpur**

**Lecture-52**
**Monte Carlo Simulations**

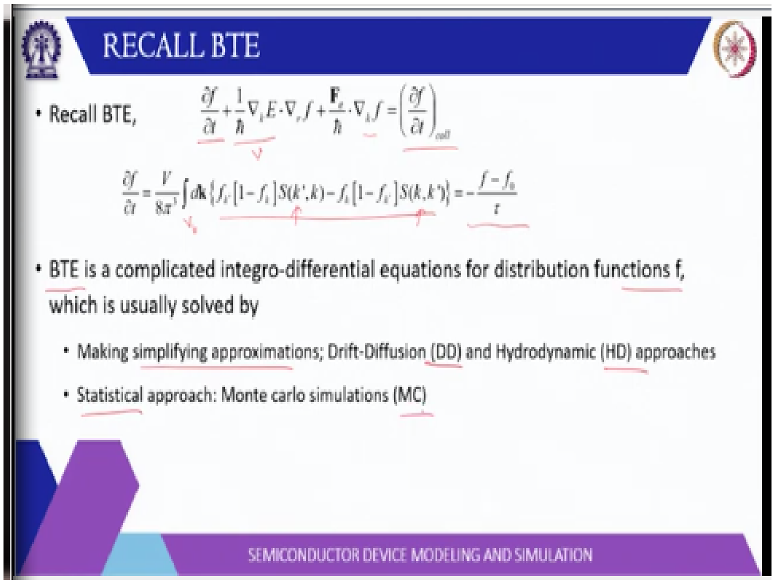
Hello, welcome to lecture number 52, in this lecture we will discuss about Monte Carlo simulations.

**(Refer Slide Time: 00:31)**




So, in Monte Carlo simulation we solve the Boltzmann transport equation by considering certain number of carriers and then tracking them basically. So, subjecting them to different scattering events and then tracking them over a period of time, we can obtain the parameters related to that particular material.

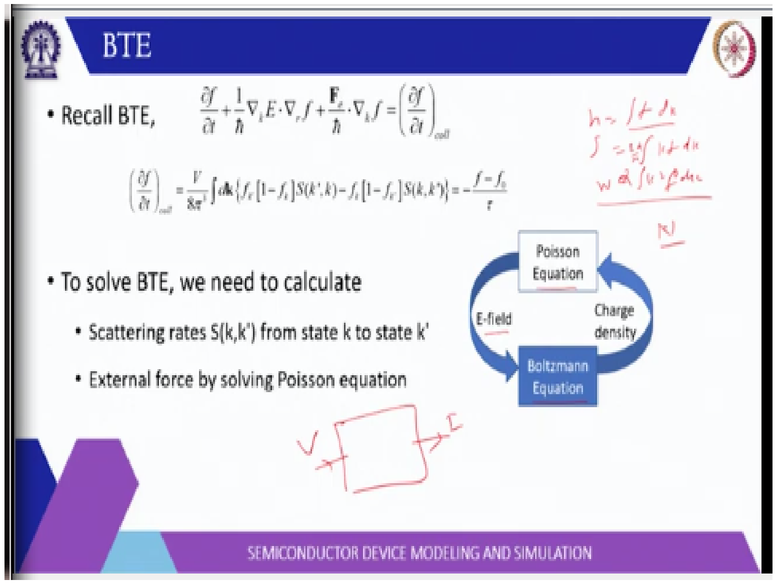
**(Refer Slide Time: 01:02)**




So, if you recall the Boltzmann transport equation, so del f by del t is a time derivative then del E y del k by h bar is the velocity times del f by del r. Then plus external force that is dp by dt and this is del f by del k which is same as del f by del p = del f by del t due to collisions. And del f by del t can also be expressed as the integral of these different or summation of over all the scattering mechanisms, so that is integral over V k prime V k.

And then f k prime times 1 - f k s k prime this is a probability of scattering from k prime to k and this is a probability of scattering from k to k prime. And this is approximated as -f - f naught by tau, whereas tau is the corresponding relaxation time. Now we know that Boltzmann transport equation is fairly complicated integral differential equation to solve for the distribution function f, so what we do? We either make some simplifying approximations then we have Drift-Diffusion model and hydrodynamic approaches or we can use statistical approach that is Monte Carlo simulation.

**(Refer Slide Time: 02:26)**

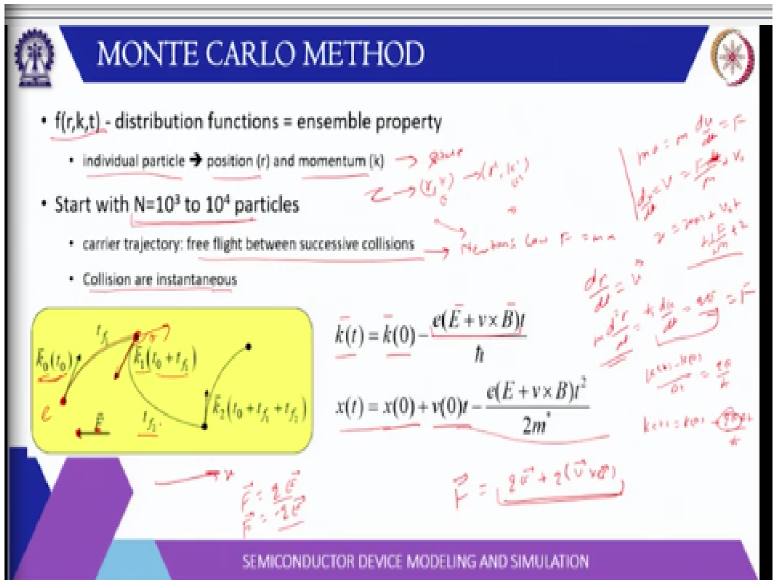



In Monte Carlo simulation you want to solve for at the end of the day what do we want? We want the I V characteristic, so given a potential V what is the current I that will flow through the device basically. So, when you apply the voltage these charges get disturbed and this imbalance in charge create some electric field and that is obtained by solving the Poisson equation. Then this electric field is a driving force of the current then we solve the Boltzmann transport equation to find out what is the new carrier density?

What is the current density? What is the energy density and so on? Now if you look at it although we can solve for the distribution function f but generally we solve in terms of the moments of function f. So, for example n is integral f over dk, so there is a moment first order. So, this is average of F and there is a carrier condensation. Similarly j is related to integral k f dk, so with some factor q h bar by m. Then similarly energy also, it is related to k square f dk, so we solve for these moments basically.

Now in Monte Carlo method we have n number of particles and we subject them to scattering events and the applied field then we track them to obtain the how their velocity actually change or what is their final step as a function of time.

**(Refer Slide Time: 04:16)**




So, let us consider distribution function and this distribution function is the combined property of all these carrier's ends. And generally in Monte Carlo we stick somewhere range 10 raise to 3 to 10 raise to 4 particle we consider because if we use less number of particles then we will not be able to capture the statistical property or the average property. If you use too many particles then the timing will be too much, so it will take lot of time, so it may not be practical.

So, what is done here? For individual particle that means all these 10 raise to power 4 particles their position are and the momentum k constitutes a state. Then there is a scattering time that means there is a probability associated with each particle that it will undergo scattering or not. And it goes under scattering then it is position r and the momentum k changes to r prime k prime and energy changes to E to E prime, so the state is basically changing due to these collisions.

Now all these carriers will not go through the scattering at the same time because there is a probability. So, some of them will go scattering at t some will go at t + delta t and so on. So, during between the 2 scattering events they follow the normal path, so there is a free flight between the successive collisions, and this is basically taken care of by Newton's law F = ma. And of course for the collisions we assume that they are instantaneous.

Although there are some finite time is there but there is pretty small and we can assume that the collisions are instantaneous. For example, let us say there is a position here at t = 0 this wave vector is k 0, then it let us say the electric field is in let us say this is x direction, so the electric field or the corresponding F is in - x direction. So, F is the force then see let us say it is carrier is if it is whole then force = q times E and if it is electron then force = -q times E.

So, if you consider this as a whole then electric field will also in -x direction and if this is electron then the force is opposite to the electric field. And due to this field let us say F these electrons get accelerated, so this electron moves opposite to the electric field basically. So, let us say this is electric field now and these are the electrons, so these are electric field. Now initial at t = 0 they have some wave vector k 0.

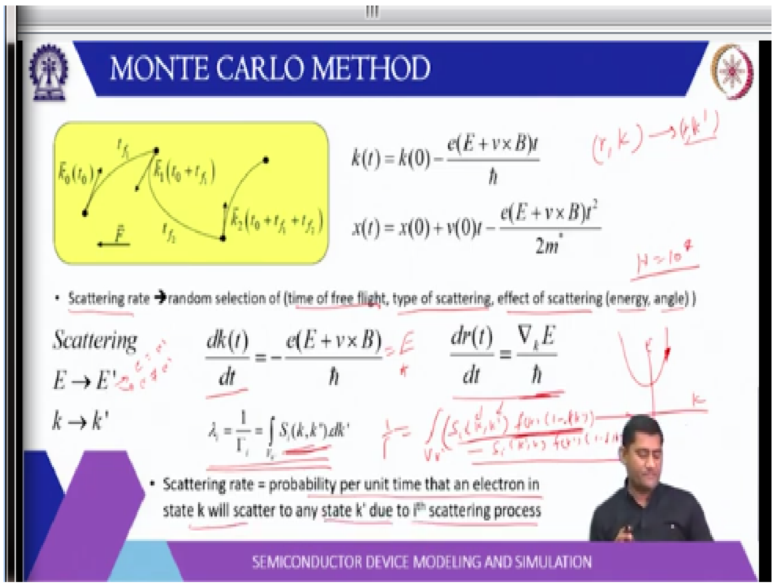
So, we can write the equation dr by dt is the velocity and d 2 r by dt square m or you can write dp by dt which is h bar dk by dt is the force. So, if you consider this force equation dp by dt = qE from this you can write k at time t - k at 0 divided by delta t = qE by h bar. So, from this you can find out that k at t = k at 0 + qE delta t by h bar. So, q is a force now if you have magnetic field and so on then you can use a general expression for the force that is general force on electron is q times E if q is the charge plus q into V cross B.

So, total force, so we can substitute this q by the total force here, so this is for electron q because –E, so -E times E + v cross B, and E and B are the vectors basically, this k is also vector. So, during the free flight time we can follow this equation that means the k is changing linearly. So, the wave vector k or momentum is changing linearly with time, what are the positions? Because d 2 r by dt square is the force, so this let us say we can write a force here so dr by dt is force time t plus some constant the initial velocity.

So, you can write let us say this is m a you can write m times dv by dt = force. So, your V = F dt by m + v naught, so F t by m + v naught. Then this is dx by dt, so again you integrate then x is becomes x naught + v naught t + F by m half t square, so the t becomes t square by 2. So, your x is given as x 0 + v 0 t + force - e times E + v cross B t square by 2m. So, here you see the equation of the position is parabolic.

So, that means during the free flight time these electron do not move in a straight line but they follow some kind of parabolic relationship till they encounter another scattering event. So, this is the direction here, then after scattering the direction change, so this is a scattering angle theta and now new state here is k 1 at t 0 + t f 1 and so on. So, the free flight time t f 1, t f 2 can be different they need not be same because it depends on the probability of a scattering.

**(Refer Slide Time: 10:51)**




Now if you consider the scattering rate, so in the scattering rate we have to select the time of free flight that means after how much time this electron will undergo the scattering. Then it will undergo what type of scattering and what is the effect of that scattering? So, whether it is elastic or whether energy will change or whether it is isotropic or non isotropic how the angle will change, so this we have to decide.

So, for scattering plus energy changes from e to E prime, so for elastic E = E prime for elastic E will not be equal to E prime. And then k will change will as a k prime and dk by dt is given by this force by h bar and dr by dt is basically depends on the band structure, so this is a velocity. See the velocity of electron is determined by it is state basically, so if you consider E-k diagram or these electrons are in certain band then let us say this is a k.

So, from the k you can know what is the velocity of this electron, now this velocity is actually a group velocity and that is the velocity that is of concern to us. So, velocity then the force and the scattering, so scattering we know if you recall the general expression for the scattering is integral over V k prime, so over the volume k space. Then all the integral mechanisms sum over all this let us say ith scattering event, so the probability of scattering from k to k prime is f s k comma k times f k times 1 - f k prime.

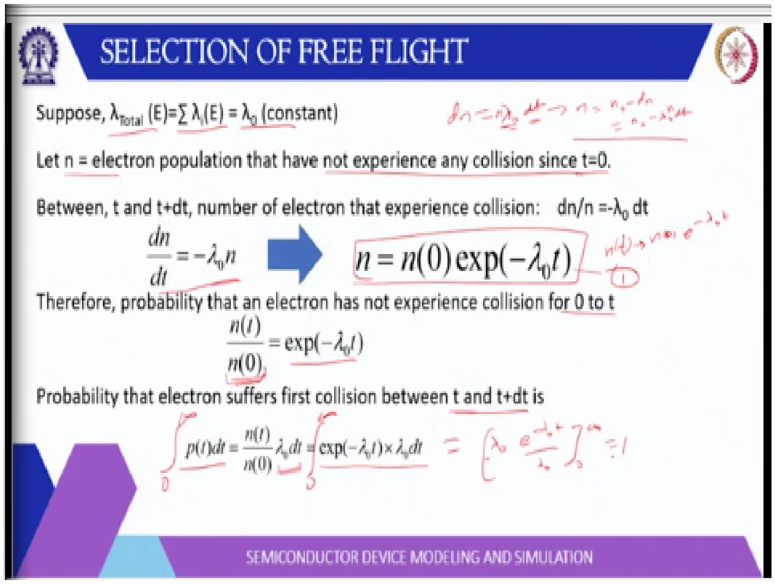
Then of course you have to have minus the negative scattering rate, so that is s i k prime comma k times f of k prime times 1 - f of k, that is integrated over k prime. So, this is the expression. Now what we are doing here? We are considering individual carriers, so we do not have to write whole equation, we have to only consider the particular scattering of a particular carrier. So, this is basically scattering out then there are other carriers we are considering n equal to let us say 10 raise to power 4.

So, some of this carrier will be in k, some of them will be in k prime and so on. So, both scatterings are actually considered, so you do not have to consider the whole expression just the individual scattering from k to k prime we have to consider. Then this has to be multiplied by f of k times 1 minus say f of k prime. So, if you assume that f of k prime is 1 - f of k prime, so that also we do not have to consider because here we are considering individual carrier.

So, this f will not actually come into the picture here. So, this is scattering rate for this individual carrier is simply S k to k prime dk prime. So, what is the probability of a electron in state k at position r? What is the probability it will scatter to k prime? Again it is as the same position; position does not change instantaneously. So, the same position it will scattered to k prime, so what is the probability?

And that is given by scattering rate S and S i is the scattering due to ith mechanism. So, there may be multiple scattering mechanisms, so if that scattering mechanism is present at that particular position or it is influence is there then it will scatter, so it is all probabilistic basically. So, that is how the scattering rate is calculated for individual carriers. Now scattering rate is the probability per unit time that electron k state will scatter to any state k prime due to ith scattering process.

**(Refer Slide Time: 14:50)**




Now how do we select which scattering process and how we select the free flight time? So, let us assume we as add all the scattering mechanism and that is lambda total. And we assume that this is equal to lambda naught, so lambda naught is the total scattering rate due to all the scattering mechanisms. So, that means we will consider these scattering for all the carriers. Now let us say n is the number of electrons that have not experienced any collision till time t from t = 0, since t = 0 they have not experienced any collision.

Now because lambda naught is the scattering rate, that means number of electron let us say dn that will experience the scattering will be lambda naught dt because dn by dt is -lambda naught. Now what will happen? After the scattering for time delta t, n will become n naught - dn, so that will be n naught - lambda naught dt. So, from this you can write dn by dt is -lambda naught times n, so this is lambda naught n, this is should be lambda naught times n.

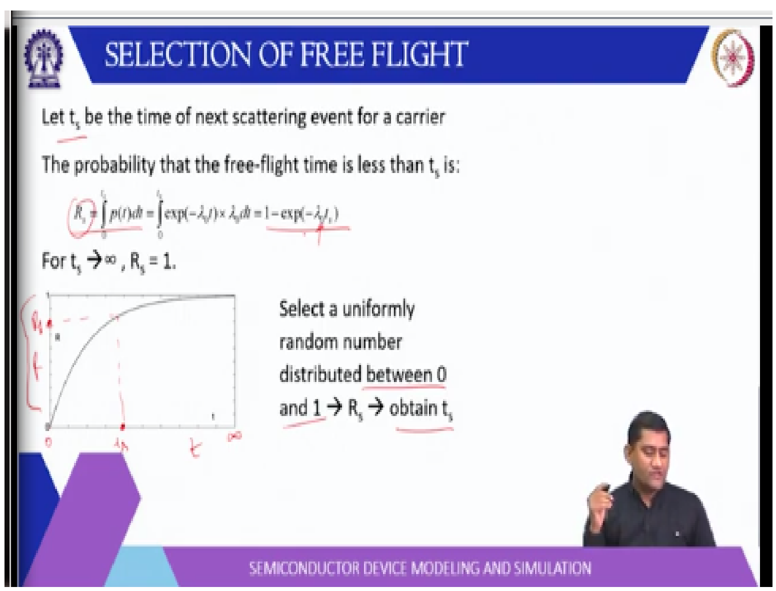
Because lambda naught is the scattering rate, now there are n number of carriers, so they are equally probable, so n lambda naught is a scattering rate, so it will be n lambda naught dt. So, dn by dt is -lambda naught times n, so with time the number of electron that have not experienced any collision is decreasing basically. Then of course if you solve it dn by dt = -lambda naught n and then integrate you will get n = n naught exponential -lambda naught t.

So, at given time if you consider with respect to t = 0 the number of carriers that have not experience the collision is n naught, the number of carriers which has not experienced the collision at t = 0 times e to the power -lambda naught t. Now therefore the probability that electron has not experienced any collision from 0 to 2 is -exponential lambda naught t, so that is n t - n at 0.

So, number of collision free electron at t = 0 in the denominator, number of collision free electron at t = t that ratio is a probability and that is by this equation, let us say equation 1 is e to the power - lambda naught t. Now what is the probability that these carriers will suffer their first collision at t between t and t + dt? That is you have to multiply this probability by scattering rate in the time duration delta t.

So, if lambda naught is the scattering rate then lambda naught dt is a scattering basically. So, probability of collision between t + t dt is n t by n naught **x** times lambda naught dt which is exponential -lambda naught t times lambda naught dt, so that is a probability of collision between t and t + delta t.

**(Refer Slide Time: 18:32)**

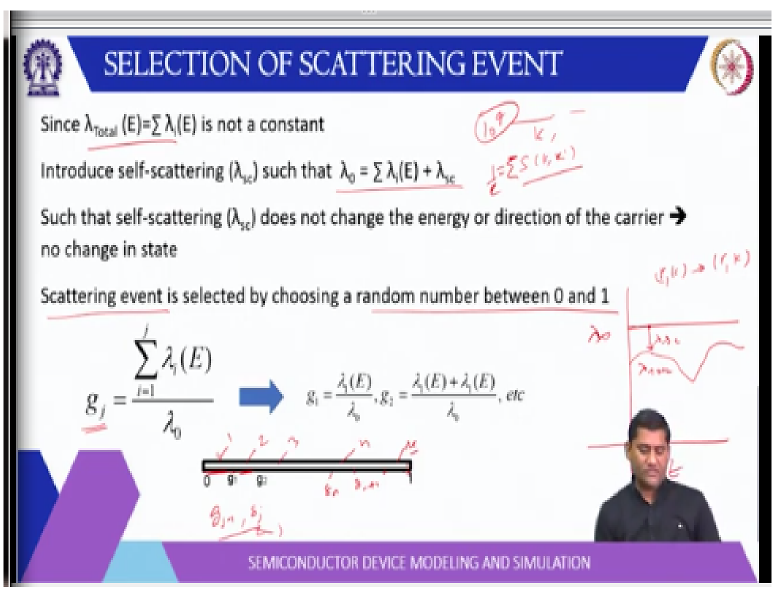



Now if you integrate this one let us say 0 to Infinity what will you get? You will get lambda naught exponential -lambda naught t by lambda naught and this is 0 to infinity. And if you see it at 0 this is exponential 0 is 1, so this is 1 and this will be minus actually, infinity will go to 0, so this will be 1. So, that is perfectly ok because the probability from 0 to t = infinity should be 1. And in between it will be between 0 and 1, so this probability will vary from 0 to 1.

So, this is the integral of p dt which we call as R, so this R is varying from 0 to 1 and this is the time f, t 0 to infinity. Now how do we select the next scattering time? Let us say call it t s, so let us say t s is our next scattering time. So, that will correspond to this R here, some value of R here, so what we can do? We can choose a random number R between 0 and 1. So, we can choose a random number uniformly distributed between 0 and 1 and from that R let us say this R s is the number that we got.

So, from R s we can find out the t s using this curve, so because this R s mapped to a unique t s. So, that means integrate from 0 to t s you will get 1 - exponential - lambda naught t s, that is R s. So, if you randomly select R s between 0 and 1 and then obtain the corresponding t s. So, for each carrier we can do this and because we have already included this lambda naught, so that means it has already accounted for the overall scattering rate.

**(Refer Slide Time: 20:28)**




Now another question may arise how do we select which scattering mechanism we should use? And also another question because all these 10 raised to power 4 carriers, their states are changing with time, so that means and this S is function of k comma k prime is a sigma k comma k prime is 1 over tau. Then this is function of this wave vector, so this is a scattering rate may also change basically, so lambda total may not be equal to lambda naught.

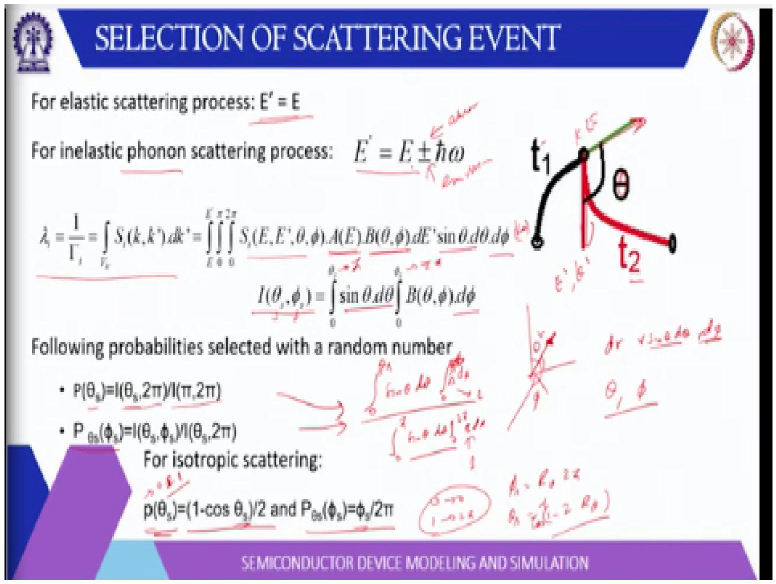
So, to make it equal to lambda naught what we can do? Let us say this is your lambda naught and as a function of time the scatting rate may be something like this sometimes they sometimes like they are saying, so these are lambda total. So, that means there is a difference between lambda naught and lambda total the actual scattering rate, so this difference we can as call self scattering. Say that means this many carriers will not undergo any scattering but when the scattering is applied to them they will be self scattered.

That means their position R moment wave vector k will be replaced by same position in the wave vector k, so there will not be any change that is self scattering. So, this is a fix self scattering to make sure that total scattering rate is lambda naught constant and we can use the model e to the power -lambda naught t as discussed in the previous slide. So, now this scattering event is selected by choosing a random number again between 0 and 1. And what we can say?

That number if it falls between g j - 1 and g j then we will assign a scattering rate j, so this will be scattering rate 1, so scattering event will be 1, 2 and even 2, 3 and so on. Let us say this is nth 1, so this will be g n + g n + 1 usually g n and this may be some self is scattering maybe here, self scattering. So, we select n number between 0 and 1 and then we find out in which reason it falls, so it also takes care of the probability, let us say some event are more probable one.

So, then they will take a bigger chunk of line space here, some events are less probable, so they will take a smaller chunk of space here. And let us say this lambda total touches lambda naught then lambda c will be 0, so then this will be very small, so this will be close to 1 only. So, that way we can select the free flight time and then we can also choose what type of scattering event will be followed.

**(Refer Slide Time: 23:13)**




So, now for elastic scattering there is no change in energy. So, before the scattering and after the scattering both the energies are equal. And for n inelastic scattering especially using the phonon they can emit a phonon or they can absorb a phonon, so this plus sign that means energy is increasing, so that is absorption of a phonon. And energy is decreasing E - h bar omega that means they are emitting a phonon.

And then if you recall that scattering rate is integral S dk prime over the volume k prime then that can be written as some psi times some coefficient of energy, some coefficient of theta and phi we are using basically spherical coordinate r, theta and phi. So, let us say this is initial k 0, let us say this is k here and this is the perpendicular angle, this is after scattering, so this scattering angle is theta, so this is k, this is k prime.

And they are scattered by some angle theta the energy is E here let us say energy is E prime here, then this is a free flight time 1, free flight time 2 and so on. Now if you see here this is function of energy, this function of theta and phi they can be further breakdown. So, if you integrate in spherical domain then the integral is r dr in x direction then r sine theta d theta, so r sine theta d theta and there is a r d phi.

So, theta and phi we can separate out, so sine theta is this theta d phi is phi only, so d phi and sine theta d theta, so we can define as integral of theta and phi. Now for a individual scattering process we have to select the angle theta and phi also, they are also selected randomly. So, first you have to calculate the probability of a scattering angle theta let us say it scatters as theta s, so what is the probability?

So, that probability will be i theta s phi can be 0 to 2 pi then theta can be 0 to pi, so this maximum can be pi this can be maximum 2 pi. So, this integral from pi and 2 pi and i theta s by 2 pi, so that means it is basically sine theta d theta 0 to theta s times d phi with B 0 to 2 pi divided by 0 to pi sine theta d theta 0 to 2 pi B d phi. So, this is your probability of angle theta s. Now if you integrate it sine theta d theta is a cos theta, 0 to theta s that is 1 - cos theta and this 0 to pi is 2, so this 1 - theta s divided by 2, that is p theta.

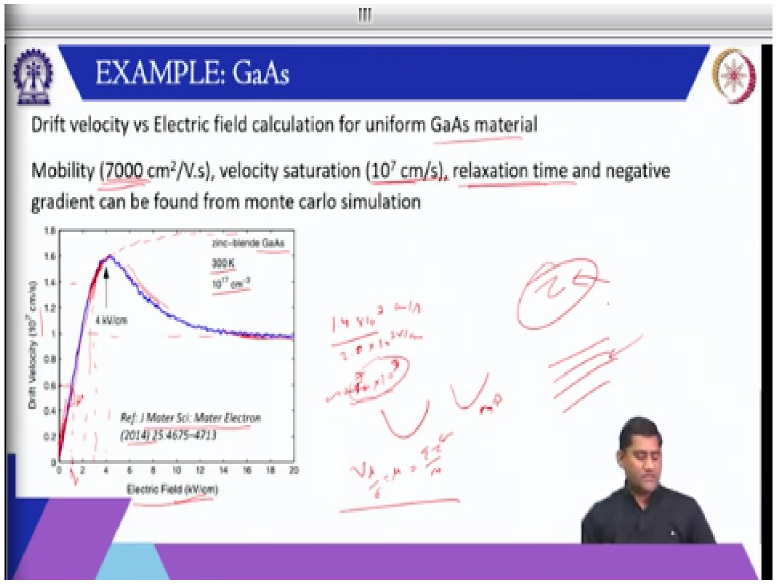
So, again we can select a random number between these limits of theta s, so this will be between maximum value of cos theta is let us say theta is 0 to pi. So, cos theta will be 1 or -1, so 1 means it will be 0, -1 is actually 2, so this p theta is again will be between 0 and 1. So, we can select a random number between 0 and 1 and then corresponding to that random number we can calculate that theta s.

Similarly probability of phi s for given theta s, so that is i phi s divided by i 2 pi, so this is the same thing. Now given theta s with 0 to phi here and 0 2 pi here, so that is your second probability. So, this also phi s if you integrate it is 0 2 pi is 2 pi only if you assume that B is 1 here, this is let us say 1. So, up to phi s it is simply phi s, so the probability is phi s by 2 pi. So, again a random number can be selected between 0 and 1 and it can be scaled accordingly, so 0 correspond to 0 and 1 correspond to 2 pi.

So, accordingly you can multiply that number by phi s by 2 pi, so probability into 2 pi will be your phi s. So, you select a random number, so phi s is that random number phi times 2 pi and your theta s is 2 times R theta then cos inverse 1 - 2 R theta, R t theta is between 0 and 1. So, that way by using the random number we can find out the scattering angle and the scattering angle theta and the scatter angle phi.

And because we have already chosen the scattering process, so this E and E prime relation is divided by the scattering process itself.

**(Refer Slide Time: 28:40)**




Now this is one example from this reference general of material science 2014 paper. There they have simulated the Monte Carlo simulation for gallium arsenite under zinc blended lattice at 300 Kelvin and with toping of 10 raise to power 17 per cubic centimeter. Now if you see here the drift velocity as a function of electric field, so it basically increases up to certain point around 4 kV per centimeter and this is more or less linear.

So, that means you can define a mobility here and if you see the mobility let us say this is 1.4 divided by 2.5, so 1.4 into 10 raised to power 7 divided by 2.5 10 raise to the power 3 volt per centimeter and this is centimeter per second. So, if you get it the mobility that will be around 10 raise to power 4 1.4 by 2.5, so that roughly comes around 10 raise to power 4 into 1.4 by 2.5. So, 125 then 15.5. So, around 5.6 10 raise to power 3.

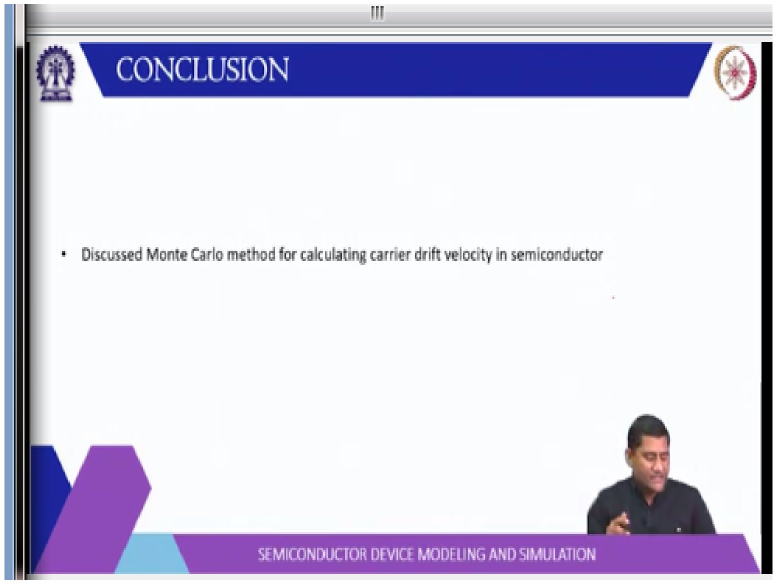
So, here it is basically getting 7000, so it may not be 2.5 maybe you will say 2, so let us it is 2 somewhere here, then it goes to 7000 that makes sense. So, 7 10 raise to power 3, so that tells you around 7000 centimeters per volt second. Now you notice one more thing here this slope actually changes, see here the slope is high, here the slope gets reduced, so that is why we are kind of over estimating here.

But if you use closer by let us say this region here 0.6 to let us say 1 here, this is 1, so that gives you around 6000 centimeter square per volt second. So, this is a basically mobility but if you go here the mobility will tend to decrease because we are reaching the saturation region. But if you see here this is a negative gradient that we have already discussed, what is happening here? From gamma valley they are going to the satellite valley where the mass is actually more, so this velocity is small here.

Now saturation velocity you can see here is order of 10 raise to power 7 centimeter per second and from this v d by e, you have mu here which is q tau by m. So, if you know the effective mass, you can also estimate the relaxation time and this kind of simulation can be done with the Monte Carlo method. And these are done for different materials to estimate these parameters what is the mobility? What is the saturation velocity and what is the relaxation time?

And they perfectly match with the experimental data and now this method has been very useful in generating such type of datas basically another thing if you recall the hydrodynamic model, we assume some relaxation time but we did not know how to get that value. So, that values are actually obtained from the Monte Carlo simulation of these individual materials and then for multi layered structure for each material these Monte Carlo simulated values of scattering are actually a relaxation time are used in the hydrodynamic simulation.

**(Refer Slide Time: 33:30)**




So, in this lecture we have discussed the Monte Carlo method for calculating the carrier drift velocity in the semiconductor. Starting with the considering the number of carrier then estimating the scattering probability, scattering time, free flight time then scattering mechanism, then for each scattering mechanism what is a theta, what is the phi angle of scattering. Then with that estimation when we follow it over a time and for each time we plot what is the state of these carriers.

And once there is a steady state we have some kind of overall state of these carriers because under constant electric field this carrier will finally scattered to some steady state characteristic. So, that steady state a characteristic is plotted here, so you consider 1 electric field apply this Monte Carlo method, find the steady state and plot it here. So, this is basically done for all these electric field individually. And that we can estimate the transport properties of individual material, so thank you very much.