Semiconductor Device Modelling and Simulation
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Lecture - 36
Semiclassical Transport (Continued)

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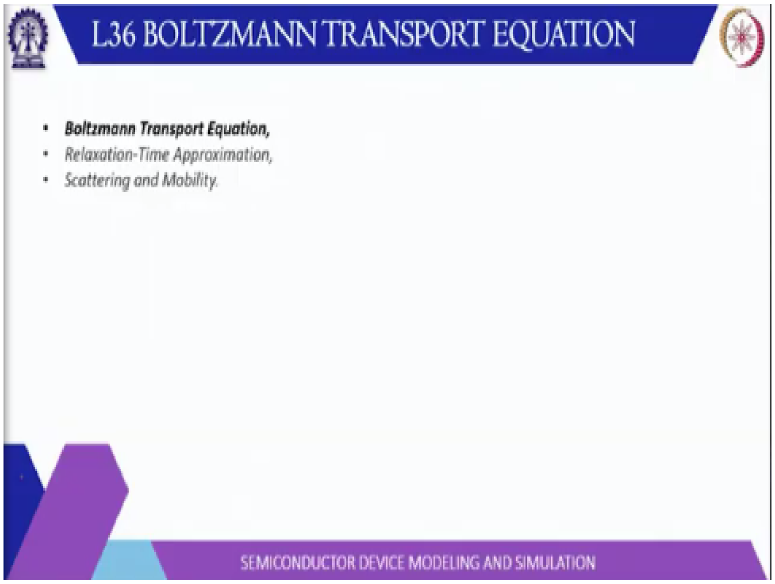

L36 BOLTZMANN TRANSPORT EQUATION

- ***Boltzmann Transport Equation,***
- *Relaxation-Time Approximation,*
- *Scattering and Mobility.*

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Hello welcome to lecture number 36 let us continue our discussion on semi classical transport. So, in today's lecture we will discuss about the Boltzmann transport equation. Boltzmann transport equation is actually equation which basically solves for the; or it basically explains how the distribution function will behave with respect to the position time and the momentum.

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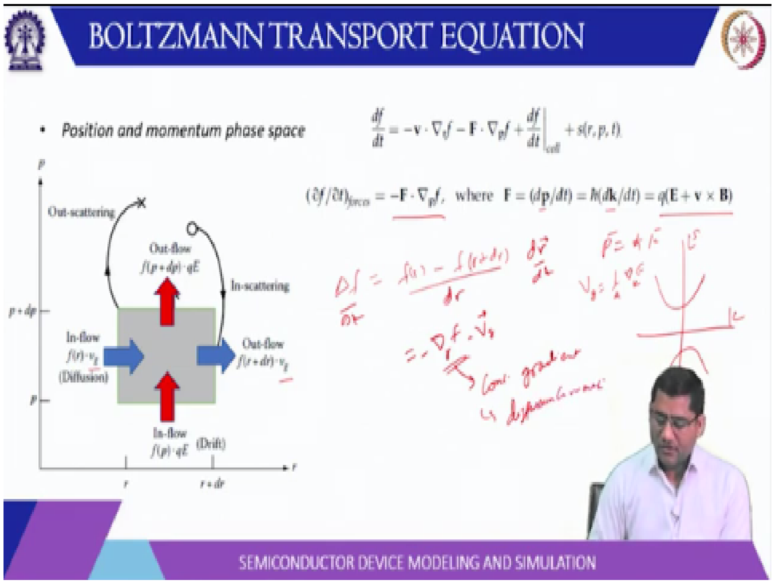

BOLTZMANN TRANSPORT EQUATION

- *Position and momentum phase space*

$$\frac{df}{dt} = -\mathbf{v}\cdot\nabla_r f - \mathbf{F}\cdot\nabla_p f + \left.\frac{df}{dt}\right|_{coll} + s(r,p,t)$$

$$(\partial f/\partial t)_{force} = -\mathbf{F}\cdot\nabla_p f, \quad \text{where} \quad \mathbf{F} = (d\mathbf{p}/dt) = \hbar(d\mathbf{k}/dt) = q(\mathbf{E} + \mathbf{v}\times\mathbf{B})$$

$$\frac{\Delta f}{\delta r} = \frac{f(r) - f(r+dr)}{dr} \quad \frac{d\vec{r}}{dt}$$

$$= -\nabla f \cdot \vec{v}_g$$

↳ conc. gradient

↳ dispersion

$\vec{p} = \hbar\vec{k}$

$v_g = \frac{1}{\hbar}\nabla E$

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So, let us consider phase diagram so phase space basically here phase space we refer to momentum and position. You can include time also but let us keep time away for time being. So, this is a phase and momentum so how the distribution function f is changing with respect to phase and momentum. Now let us say here x axis is the r the position and y axis is the momentum p.

And let us consider a small box here where we are monitoring the function f or distribution function f. So, just to recall that f is the probability of finding particle with position r momentum p at a given time t so, f in general is a function of position which is a vector momentum which is a vector and time. So, of course this can also be written r x, r y, r z and similarly p can return as p x, p y, p z so there are total seven variables.

In a crystal this f basically evolves as a function of time. So, even if you do not apply any force or this is an equilibrium some kind of scattering will go on. And in equilibrium what will happen? There will be detailed balance basically each process will be balanced by equal and opposite process. So, if some carriers are moving from f to let us say f + p + delta p then similar number of carry will come from p + delta p to p and so on.

Or they may move from p 1 to p 2 or r 1 to r 2 so same will come back to the same so that the distribution remains the same. Now here if you look the flow of these particles so along the y axis at the lower point it is f p so this position is p then at higher p + delta p it is f p + delta p. Now momentum will change due to certain force so in general force can be due to electric field which is q E plus the force can be due to magnetic field.

So, that is q times v cross b so, here for simplicity let us use keep force = q E. So, if you want to find out the change along this momentum axis, we can write the number of particles or the probability of particles that are entering. So, that will be f p then particle that are leaving that will be f of p - p + delta p so, this is the net particle that are entering. So, this can be written as if you divide by delta p and if you multiply delta p.

So, this is basically the derivative del f by del p with a negative sign times del p. So, this is basically your delta f so this is your delta f and if you divide by time delta t so this change over time then you can write this as and because p is a three dimensional variable. So, you can instead of write del p del f by del p we can write minus del of f with respect to p then delta p by delta t and Newton as del p by del t.

Now del p by del t is force basically so this is minus del p f times force and force is this q E + v q times v cross b. So, your delta f by delta t in momentum direction is the gradient of f with respect to p times force. So, this is the expression - f dot del p where f is dp by dt and this is q times E + v cross b. Now this force is related to momentum v p and we know for the crystal electron p = h bar k where k is the wave vector and p is the crystal momentum.

Actually, electron momentum will be different but this is the you know moment of that electron encounter in the crystal and according to the band structure this is the say E k diagram. So, this is the bandage structure if it is parabolic then of course we can also define the effective mass and all. Now let us consider along the x axis so similarly we can write the change in distribution function will be f of r - f of r + delta r, this is the total number of you know particles you can say entering in this region.

And their velocity is basically v g which is the group velocity and you can recall from a band diagram if they obey the parabolic bandage structure you can write v g = 1 over h bar del E by del k there is a group velocity. Now similarly we can divide this by delta r or you can write d r times d r here and if you divide by delta t then you have d t, here so, this is basically your gradient of, f with respect to r with a minus sign times dr by dt and dr by dt is basically group velocity.

So, times group velocity, so the change in the distribution function along the position is again the gradient of, f with respect to position times the group velocity. Now here you can see that gradient of distribution function with respect to position is actually telling you something about the concentration gradient. And that basically correspond to diffusion current.

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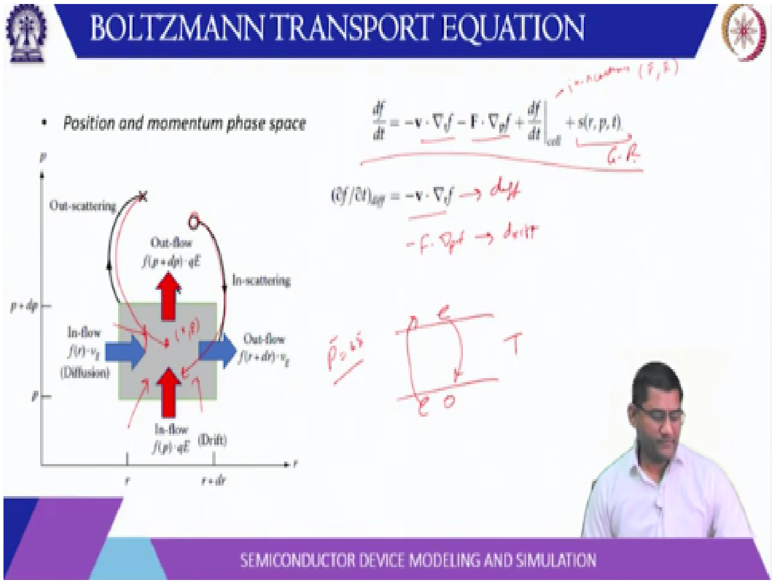

BOLTZMANN TRANSPORT EQUATION

- *Position and momentum phase space*

$$\frac{df}{dt} = -\mathbf{v}\cdot\nabla_r f - \mathbf{F}\cdot\nabla_p f + \left.\frac{df}{dt}\right|_{coll} + s(r,p,t)$$

$$(\partial f/\partial t)_{diff} = -\mathbf{v}\cdot\nabla_r f \rightarrow diff$$

$$-F\cdot\nabla_p f \rightarrow drift$$

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So, we have two terms basically here one is gradient along the position axis another gradient along the momentum axis. So, this term basically correspond to the diffusion and this - F dot del p f this one correspond to the drift. If we assume the selective field is there so this is a drift due to the electric field. Now you notice here what we have done we have included that this is the number of particles that are entering this space.

So, net number of particles that are entering the phase space. Now it is possible that if there is a particle here it can just get scattered to outside or if there is a particle outside it can get scattered inside. So, we can write another scattering term. So, this will be net in scattering so this will be net in scattering. So, this is basically means the all the particles that are scattering to position r, p or we will use p and k interchangeable because p = h bar k in crystal.

So, in scattering to position r and vector k, then of course you can have another term which could be due to the generation of the carriers inside the semiconductor if you recall that at a given temperature electrons in the conduction band in the balance band have a probability to go to the conduction band thus create electron hole pair. So, these are net generations of this electron they can of course recombine also.

So, this s is basically generation minus recombination and this overall equation is basically specifying what is the rate of change of this distribution function f.

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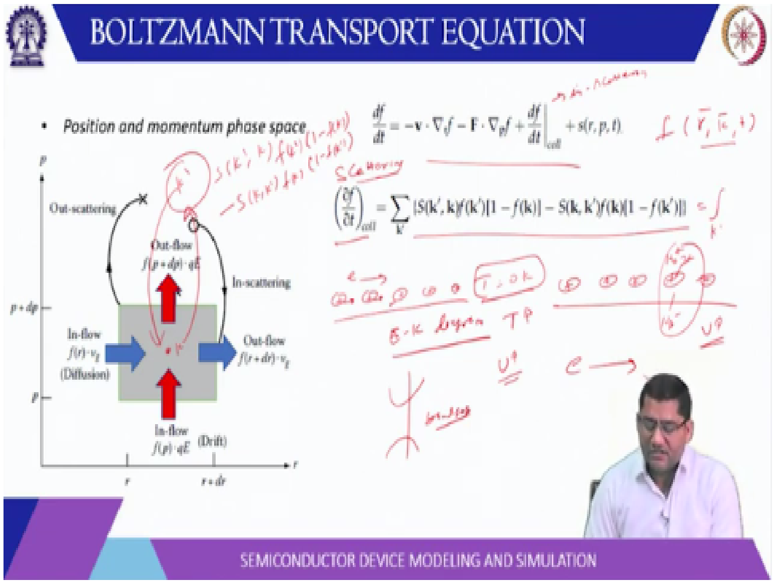

BOLTZMANN TRANSPORT EQUATION

- Position and momentum phase space

$$\frac{df}{dt} = -\mathbf{v}\cdot\nabla_r f - \mathbf{F}\cdot\nabla_p f + \left.\frac{df}{dt}\right|_{coll} + s(r,p,t)$$

$$f(\bar{r}, \bar{k}, t)$$

Scattering

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \sum_{k'} [S(\mathbf{k}',\mathbf{k})f(\mathbf{k}')[1-f(\mathbf{k})] - S(\mathbf{k},\mathbf{k}')f(\mathbf{k})[1-f(\mathbf{k}')]] = \int_{k'}$$

$$S(k',k)f(k')(1-f(k)) \quad -S(k,k')f(k)(1-f(k'))$$

T = 0 K

E-K diagram

TP

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Now let us look further look into this scattering term. Scattering is an important event that takes place inside the semiconductor or any other material. This scattering can be due to multiple factors so for example inside the lattice these are the basically atoms or nucleus that are sitting there and there are free electrons here, now if you look at zero Kelvin these ions are tightly fixed, they are not vibrating.

And in this situation what we do basically we solve this Schrodinger equation for the periodic crystal and we get the band diagram. So, this periodic position of these atoms is already encountered in the E k diagram. So, if you have a E k diagram for a given semiconductor then this regular positioning of these the atoms is already accounted for. So, when we write that you know this electron is moving with certain velocity.

And there are certain allowed energies some disallowed energies which are called band gap. So, this is already accounted for. Now what happens if you increase the temperature then these atoms may oscillate. So, let us say they may oscillate here other may oscillate here and so on. So, their position is now changing. Now due to this fluctuation some extra potential will come there and the scattering is due to this extra potential or you can consider another situation.

Let us say these are the ions that are situated here and then there is some other foreign atom that comes and sits somewhere here so, let us say here instead of this some z plus some or you can say n d plus or n a minus sits here so, now it will see a discrepancy with respect to the original host structure s T = 0 Kelvin. So, this is different so this difference is basically again give you some potential and which is causing the scattering.

So, by this potential if this is a charge stuff then of course there will be coulombic attraction or repulsion and if it is some other defect if it is neutral defect then due to the crystal potential variation some effect will come into the picture and there will be overall deflection or scattering. Now what these things these impurities can do let us say your electron is moving inside the crystal it will get reflected you know it may get reflected a certain angle.

Now this process can be further divided into other categories like it can be elastic process where there is a no loss of energy or it can be inelastic or it can be isotropic scattering so all those parameters. So, let us look at this dm by dt with collision. So, here we are assuming that this f is at position r wave vector k at time t. Now this is basically in a scattering. So, what is the probability this is in scattering so scattering to r and k.

So, overall scattering to r and k is basically let us say this is position k and this is some other outside is k prime. So, what is the probability that this particle will get scattered from k prime to k so, that is called that probability is called s k prime, k. So, there is a probability of scattering from k prime to k. Now if this probability is finite then we need to know whether there are carriers are there or not so, then you have to multiply by the probability of finding a carrier at k prime.

So, at k prime what is the probability that carries are there that is given by the f n for this carrier to come to k there should be vacancy this the states should be available. So, that means this would be 1 - f of k so, what is the probability that at k there is a space for the electron or carrier. So, this is basically total any scattering and then minus all the out scattering so that is probability scattering probabilities s of k, k prime.

So, that is out scattering then it will scatter only if there are electrons here so that is f of k and it will escalated two k prime if there is a empty space there so this is 1 - f of k prime so, this is a total scattering rate. Now it has to be integrated over all the k primes so this is sum of k prime or you can also write integral over k prime. So, this will be total in scattering further distribution function f and then of course this is generation net generation minus recombination.

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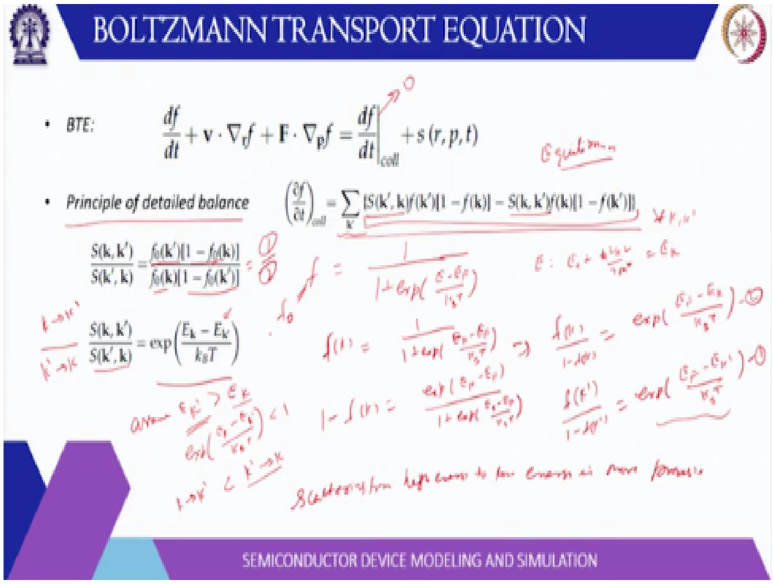

BOLTZMANN TRANSPORT EQUATION

- BTE: $\frac{df}{dt} + \mathbf{v}\cdot\nabla_r f + \mathbf{F}\cdot\nabla_p f = \left.\frac{df}{dt}\right|_{coll} + s(r,p,t)$
- Principle of detailed balance $\left(\frac{\partial f}{\partial t}\right)_{coll} = \sum_{k'} [S(k',k)f(k')[1-f(k)] - S(k,k')f(k)[1-f(k')]]$

$$\frac{S(k,k')}{S(k',k)} = \frac{f_0(k')[1-f_0(k)]}{f_0(k)[1-f_0(k')]}$$

$$\frac{S(k,k')}{S(k',k)} = \exp\left(\frac{E_k - E_{k'}}{k_B T}\right)$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

So, this is the overall Boltzmann transport equation. Now as far as scattering is concerned if you consider a situation of equilibrium. So, at equilibrium this has to be 0 del f by del t for due to collision should be 0. So, that means if you equate this to be zero then it is a sum over k prime but in equilibrium all the individual processes are balanced. So, that means this should be true for every k and k prime so, that means each term inside this summation should be zero.

So, that means if you rearrange it then the ratio of s k prime to k divided by s k to k prime will be f k prime - 1 - f divided by f of k times 1 - f of k prime. Now if you recall let us say f is some familiar direct distribution function. So, f is 1 over 1 + exponential E - E f by k T and where E is basically E c + h bar square k square by 2m effective. We can also write it let us say E k for k and k prime E k prime for k prime.

So, f of k will be 1 over 1 + exponential E k - E f by k T this is k is poles one constant then 1 - f of k will be exponential E k - E f divided by 1 + exponential E k - E f by k T and if you take the ratio f k by 1 - f k will be exponential E f - E k by k T similarly we can write for k prime so f of k prime divided by 1 - f of k prime will be exponential E f - E k prime by k T. So, this is false one constant.

Now if you look here this f of k prime by 1 - f of k prime and denominator f of k by 1 - f of k. So, that is basically this term one this is two so this is basically 1 divided by 2 and that is basically E k - E k prime so, this is exponential E k - E k prime by k T. Now if you understand that S k, k prime is the probability of scattering from k to k prime this is the probability is scattering from k to k prime to k. Now let us assume let us say k prime is a has higher energy.

So, we can say E of k prime is more than E of k that means if E of k prime is more than this then exponential of this term E k - E k prime by k B T will be E k prime is more. So, this will be less than one because this is exponential of negative term. So, this will be less than one that means the k to k prime probability is less than k prime to k probability. So, that means there is a high probability for scattering to a lower energy. So, k prime has higher energy and k is lower energy.

So, if this energy is higher then this is less than one so that scattering from k prime to case more problem. So, that means scattering from high energy to low energy is more probable and this is called principle of detailed balance. We can also listen like this now here this f 0 is written because this f is basically distribution function at equilibrium. So, generally with not f by f 0 for a distribution function at equilibrium.

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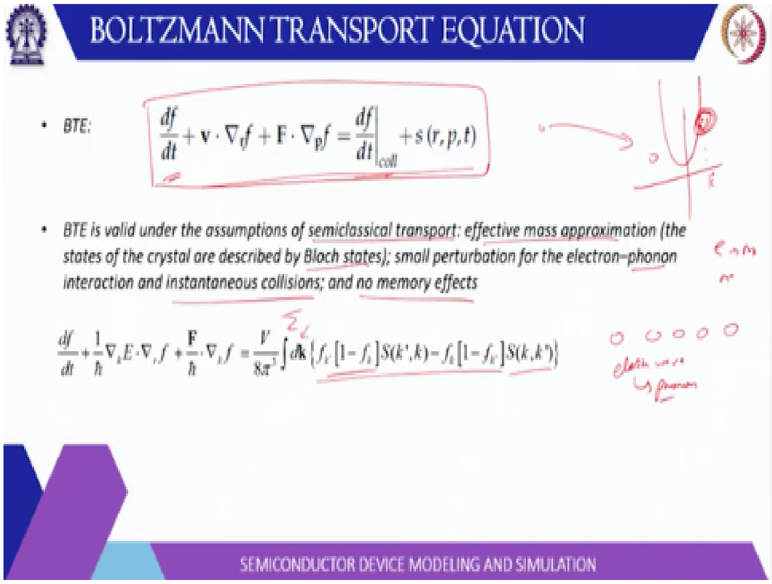

BOLTZMANN TRANSPORT EQUATION

- BTE: $\boxed{\frac{df}{dt} + \mathbf{v} \cdot \nabla_r f + \mathbf{F} \cdot \nabla_p f = \left.\frac{df}{dt}\right|_{coll} + s(r,p,t)}$
- BTE is valid under the assumptions of semiclassical transport: effective mass approximation (the states of the crystal are described by Bloch states); small perturbation for the electron–phonon interaction and instantaneous collisions; and no memory effects

$$\frac{df}{dt} + \frac{1}{\hbar}\nabla_k E \cdot \nabla_r f + \frac{\mathbf{F}}{\hbar} \cdot \nabla_k f = \frac{V}{8\pi^3}\overset{\Sigma_k}{\int} d\mathbf{k}\left\{f_{k'}\left[1-f_k\right]S(k',k) - f_k\left[1-f_{k'}\right]S(k,k')\right\}$$

elastic wave

↳ phonon

So, this is basically your Boltzmann transport equation. Now this Boltzmann transport equation is valid under the assumption of semi classical transport. So, chemical classical transport we have already discussed sound to some extent that between the scattering we assume it to be particle. And what is this particle is particle is actually a wave factor at position R and with the wave vector k. So, this is not valid, valid during the interaction.

So, when these carriers are interacting with the impurities and all they will more or less wave like they have the wave nature but when they are moving around then this wave pocket can be assumed to have a particle like nature. So, and that nature comes with a some approximation so the free electron is a mass m 0 but in the crystal this is a wave pocket. So, it is mass is effective mass so this m is replaced by m star.

So, there is effective mass approximation that takes care of the periodic potential inside the semiconductor crystal and its effect on the electron because these electrons are basically described by these wave functions that we call Bloch states. And then of course we also assume there is small perturbation of the electron phonon interaction. Now phonon is basically oscillation of these atoms the lattice atoms and that oscillation we call it elastic wave.

And the quantization of the elastic wave is called phonon and of course we also assume that these collisions are instantaneous. That means they do not go on for long time they just takes place and particle move around then of course no memory effect is included here because we assume that this del f by del t is dependent on the current position and the momentum rather than on the history of the particle.

So, there is no memory effect so under this assumption this Boltzmann transport equation is valid. And overall if you write this as integral we can write in **(()) (23:43)** root or summation so we can write it as integral also so 1 over times 8 pi q by volume then d k of course you have to include the in the 3d how this d k 4 pi k is called dk. Then these individually scattering rate n a scattering minus out is scattering.

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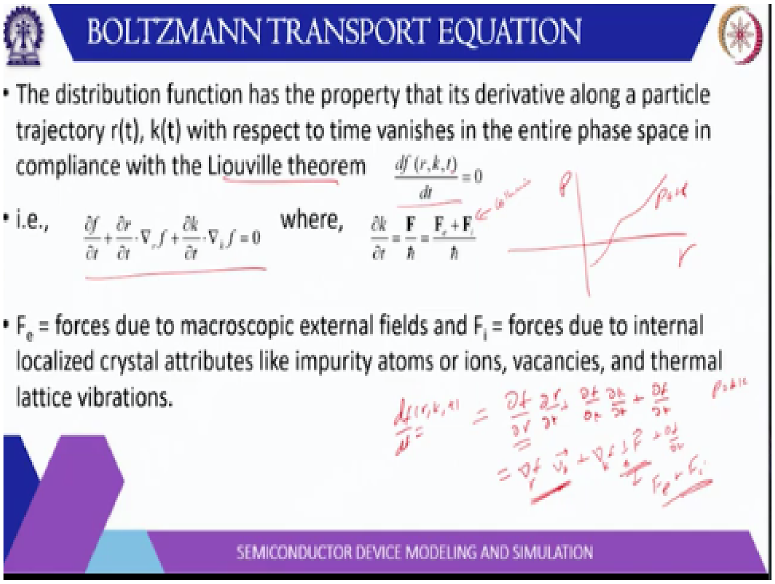

BOLTZMANN TRANSPORT EQUATION

- The distribution function has the property that its derivative along a particle trajectory r(t), k(t) with respect to time vanishes in the entire phase space in compliance with the Liouville theorem $\frac{df(r,k,t)}{dt}=0$
- i.e., $\frac{\partial f}{\partial t}+\frac{\partial r}{\partial t}\cdot\nabla_r f+\frac{\partial k}{\partial t}\cdot\nabla_k f=0$ where, $\frac{\partial k}{\partial t}=\frac{\mathbf{F}}{\hbar}=\frac{\mathbf{F}_e+\mathbf{F}_i}{\hbar}$
- F_e = forces due to macroscopic external fields and F_i = forces due to internal localized crystal attributes like impurity atoms or ions, vacancies, and thermal lattice vibrations.

$\frac{df(r,k,t)}{dt} = \frac{\partial f}{\partial r}\frac{\partial r}{\partial t} + \frac{\partial f}{\partial k}\frac{\partial k}{\partial t} + \frac{\partial f}{\partial t}$

$= \nabla f \cdot \vec{v} + \nabla_k f \cdot \frac{F}{\hbar} + \frac{\partial f}{\partial t}$

$F_e + F_i$

So, this is the overall Boltzmann transport equation there is another way to look at it as what we call as Liouville theorem it states that distribution function as a property that its derivative along a particle trajectory. So, let us say this is your phase space this is momentum p and position r and this is going through this phase space. So, along this dial along this path of this particle the derivative of this distribution function actually vanishes.

That is df by dt is 0 along the path of this particle so total derivative of df by dt can be written as df by dt now f is a function of position momentum and t. So, this can be written as del f by del r + del f by del k + del f by del t so, the overall derivative. So, del f by del r can be written as del f by del so df by dt can be done as partial derivative with respect to these three r, k and t and then df by dt so you can write del f by del r times del r by del t + del f by del k times del k by del t + del f by del t.

So, the overall derivative so del f by del r can be written as for 3d case f gradient with respect to r and del r by del t is basically the velocity plus del f by del k is the gradient with respect to k. Now dk by dt is basically your force so because momentum is h bar k so dk by dt is 1 by h bar dp y dt so you can write 1 over h bar times f and + del f by del t. Now this due to group velocity is basically this is the concentration gradient del f by del r trans group velocity.

And then this force is of two type there can be external force and there can be internal force. Now external force is basically due to applied fields like q E or q times v cross v and internal forces are due to internal distribution of impurities or you know some vacancies or those lattice vibration phonons or defects. So, this F i actually takes care of the del f by del t due to collisions. So, that we introduce separately in the previous case. So, and then of course this has to be zero because total derivative is zero along the phase space.

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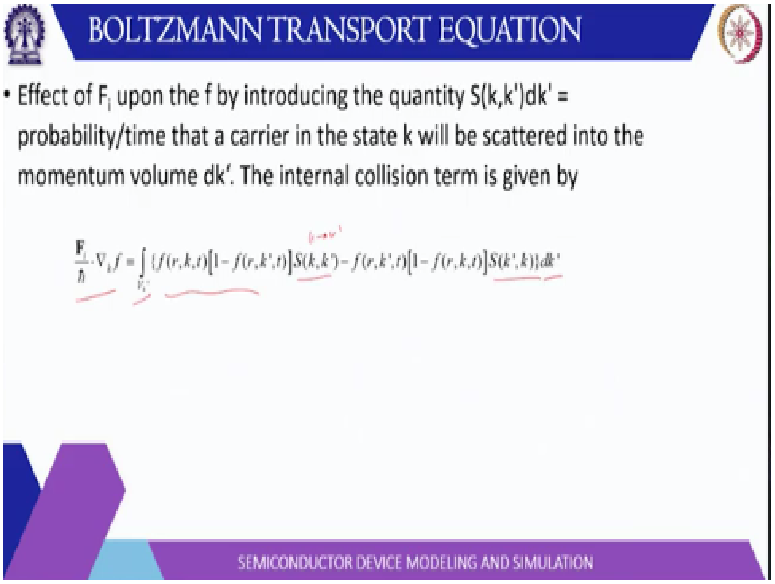

BOLTZMANN TRANSPORT EQUATION

- Effect of F_i upon the f by introducing the quantity S(k,k')dk' = probability/time that a carrier in the state k will be scattered into the momentum volume dk'. The internal collision term is given by

$$\frac{\mathbf{F}_i}{\hbar}\cdot\nabla_k f = \int_{V_{k'}} \{f(r,k,t)[1-f(r,k',t)]\overset{k\to k'}{S(k,k')} - f(r,k',t)[1-f(r,k,t)]S(k',k)\}dk'$$

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Then here if you notice that this is these two forces come together so they are on the same side. So, this is basically kind of out scattering so F i by h bar del f by del k is the outer scattering and how it is that this is S k, k prime is the probability of scattering from k to k prime and then same factor - k prime 2 k and then of course integrate over k prime all the k primes over the volume of these states with k prime.

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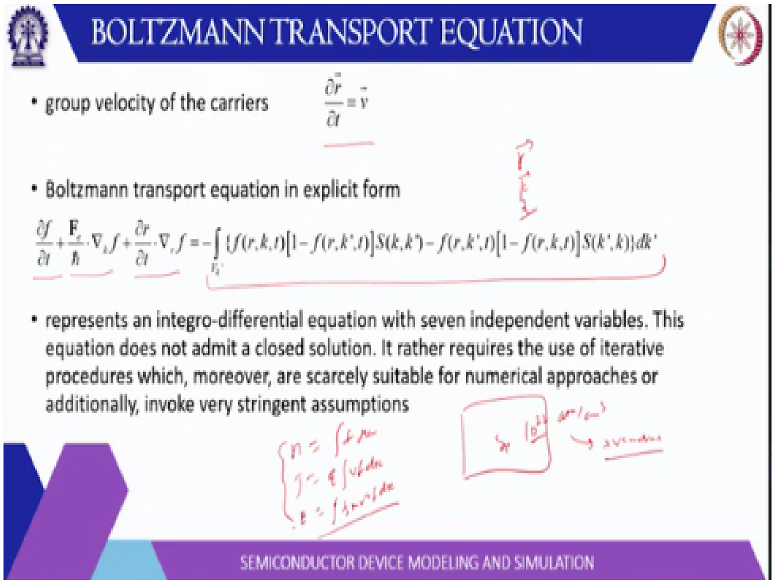

BOLTZMANN TRANSPORT EQUATION

- group velocity of the carriers $\frac{\partial \vec{r}}{\partial t} = \vec{v}$
- Boltzmann transport equation in explicit form

$$\frac{\partial f}{\partial t} + \frac{\mathbf{F}_i}{\hbar}\cdot\nabla_k f + \frac{\partial r}{\partial t}\cdot\nabla_r f = -\int_{V_k'} \{f(r,k,t)\left[1 - f(r,k',t)\right]S(k,k') - f(r,k',t)\left[1 - f(r,k,t)\right]S(k',k)\}\,dk'$$

- represents an integro-differential equation with seven independent variables. This equation does not admit a closed solution. It rather requires the use of iterative procedures which, moreover, are scarcely suitable for numerical approaches or additionally, invoke very stringent assumptions

$n = \int f\, dk$

$J = q\int v f\, dk$

$E = \int [illegible]\, dk$

Si 10^{22} atoms/cm^3

→ [illegible]

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

And of course, the group velocity is dr by dt and now the Boltzmann transport can be equation can be done in explicit form where your time derivative, momentum derivative and the position derivative together and on right side we have these internal collisions term. So, this is the integral differential equation with total seven variables because r will be x, y, z then your k will have again x, y, z and the time and it is very difficult to solve.

So, now; why it is difficult to solve? Because if you consider piece of semiconductor for example; silicon there are around 10 raise to 22 atoms per cubic centimetre. So, that this many electrons will be there per cubic centimetre if each atom contributes one electron. Then even to solve for a small piece of semiconductor will you know go up was for each electron you have seven variables and this will be very voluminous.

So, what we do basically? Instead of solving for this distribution function directly which can be done for very you know cases like very restrictive cases it can be done. But in general what we do we get the moments from this equation like we discussed in the previous class from f we can get n which is integral f dk then j is integral q times v f dk and then energy is half m v square times f dk.

So, instead of using f we can use these moments and modify this equation in terms of these moments and solve for them.

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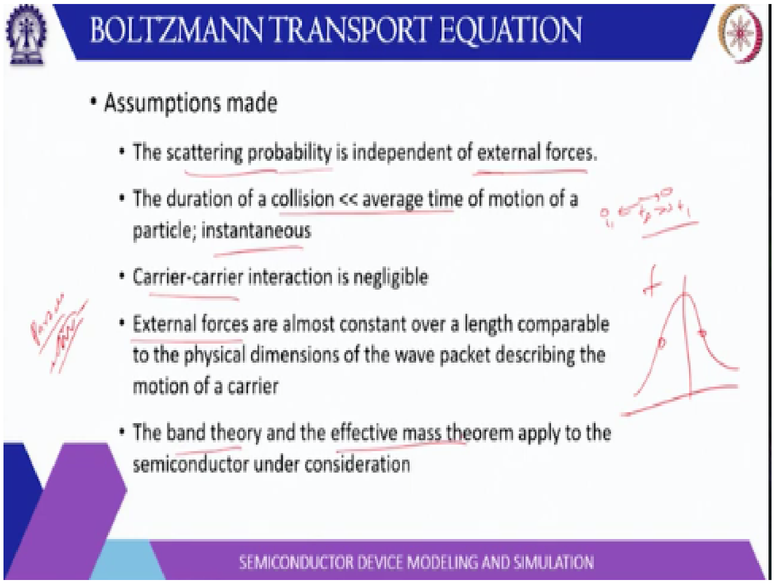

BOLTZMANN TRANSPORT EQUATION

- Assumptions made
  - The scattering probability is independent of external forces.
  - The duration of a collision << average time of motion of a particle; instantaneous
  - Carrier-carrier interaction is negligible
  - External forces are almost constant over a length comparable to the physical dimensions of the wave packet describing the motion of a carrier
  - The band theory and the effective mass theorem apply to the semiconductor under consideration

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

So, this is a typical procedure for solving the Boltzmann transport equation and these assumptions some of them we already discussed and of course other assumptions that are there. Scattering probabilities independent of the external force because we are not assuming that this probability depends on this external force. So, this internal causes are unaffected by the external force then of course these collisions are instantaneous.

So, this that means these are much less than the average time of motion. So, there is sufficient time between two collisions. So, let us say it takes some time t 1 and then for t it is free so this is mean time between collision so t f is much larger than the time for collision let us say t. So, that means they are these are instantaneous collisions in restrictive sense. Then of course we have neglected the carrier-carrier interaction.

So, we are only studying the particle f where this distribution function consists of number of particles. So, these individual particles may interact with each other but that is neglected in the Boltzmann transport equation. And then of course we have also assumed that these external forces are constant over certain length. And what is that length because we are considering this particle as a wave packet.

So, over this length of this wave packet these forces are constant because otherwise you know same particle is not experienced in the same force. And of course, we have also assumed that bend theory and the effective mass theorem apply to this semiconductor under consideration.

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CONCLUSION

- BTE derived and discussed

So, in this lecture we have drive the Boltzmann transport equations and we have discussed the physical significance of it, thank you very much.