

**Semiconductor Device Modeling**  
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**Lecture - 15**  
**Semi-classical Bulk Transport: EM field and Transport Equations**

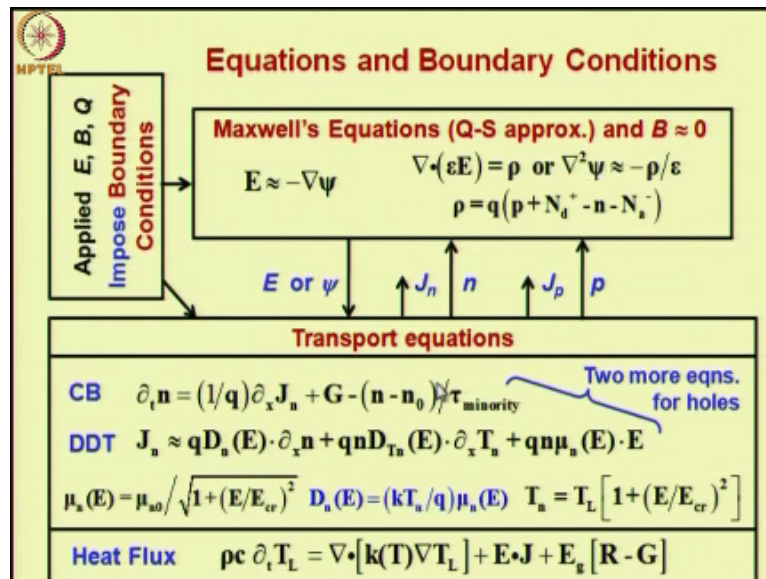
In the previous lecture, we have discussed the balance equations. We showed that the Boltzmann's Transport Equation is equivalent to infinite series of balance equation then we said however we truncate the balance equations after the energy balance equation namely that is we take only the 3 balance equation and they are sufficient to model most of the device phenomena such as velocity saturation, velocity overshoot and so on.

Now the truncation is achieved by assuming a phenomenological relation for the energy flux  $\overline{FW}$ . Now we did not give a relation for  $\overline{FW}$  because the kind of phenomena that we modeled we really did not have to use  $\overline{FW}$  and so we just left it at that. Then for these 3 balance equations namely the carrier balance equations, the momentum balance equation and the energy balance equation we showed how in practice in many situations we do not have to use all the terms of the equation.

And the equations get considerably simplified for equilibrium condition, for steady state condition and for spatially uniform conditions. So we showed how the terms drop out for these cases. Then we applied the balance equations to develop a model for velocity saturation, for velocity overshoot and for the current density expression involving drift current, diffusion current and thermoelectric current.

So this current density equation was obtained by a series of approximations of the momentum balance equation. Now let us proceed further along these lines.

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So if you summarize the result of previous in terms of the equations then these are shown here. We are already familiar with the Maxwell equations and the boundary conditions part. So let us concentrate on the transport equations. So when they use the drift diffusion thermoelectric current approximation. We absorb the balance equation result into this expression for the electron temperature and we use a field dependent mobility.

The thermal diffusivity  $DT_n$  and the diffusivity  $DN$  these 2 are expressed in terms of the mobility. Therefore, you do not need separate behaviors for  $DNE$  and thermal diffusivity etcetera. We always talk only in terms of the mobility. So you see that in the drift diffusion thermoelectric current formulation with field dependent mobility you only have 2 equations the carrier balance equation.

And the combination of momentum balance and energy balance equation absorbed into the drift diffusion thermoelectric current equation. Now you have 2 equations for electrons and 2 more equations for holes. So you see that this picture of transport equations is considerably simplified as compared to the 3 energy balance equations picture. In that picture you need 3 equations for electrons and 3 equations for holes.

So total you have 6 equations whereas here you have only 2 equations because you observe the energy balance information into the drift diffusion thermoelectric current equation. In addition to these equations for carriers or carrier fluxes you have the equation for heat flux as well.

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 **Drift –Diffusion (DD) Current Density Model**

$$J_n \approx qD_n(E) \cdot \partial_x n + \cancel{qnD_n(E) \cdot \partial_x T_n} + qn\mu_n(E) \cdot E$$

$$D_n(E) = (kT_n/q)\mu_n(E)$$

$$\cancel{D_{Tn}(E) = (k/q)\mu_n(E)} \quad \mu_n(E) = \frac{\mu_{n0}}{\sqrt{1 + (E/E_{cr})^2}}$$

Low field mobility

Approximations

4) Spatial non-uniformities of  $W_n$  in MB and  $F_W$  in EB eqns. are small, e.g.  $\partial_x W_n \ll qnE/2$

4a) Spatial non-uniformity of  $T_n$  is small, i.e.

$$\partial_x W_n \approx (1/2)kT_n \partial_x n + \cancel{(1/2)kn \partial_x T_n} \text{ or } \partial_x T_n \ll (T_n/n) \partial_x n$$

Now let us look at the drift diffusion current density model. This is the further approximation of the drift diffusion thermoelectric current expression. So here you find that the thermoelectric current term is neglected and so correspondingly you do not require the expression for the thermal diffusivity. Now the series of approximation for achieving this are the same as the approximations that we did for drift diffusion thermoelectric current plus an additional approximation related to the gradient of the carrier temperature.

So, these are the approximations listed here. So first let us repeat the approximations of the drift diffusion thermoelectric current model and then at the approximation of the temperature gradient. So quasi static approximations of the momentum balance equations then thermal energy of electron is assumed to be much greater than the drift energy. Quasi-static approximations of the energy balance equation, spatial non-uniformity of  $W_n$  in momentum balance equation and  $F_W$  in energy balance equations are small.

This is assumptions that we had make. The additional approximation that we are now making to get the drift diffusion model is that of the related to the spatial non uniformity of the carrier temperature  $T_n$ . So we say that spatial non-uniformity of  $T_n$  is small that is this term in the gradient of the kinetic energy is neglected which depends on the temperature gradient. In other words,  $\partial_x T_n / T_n \ll \partial_x n / n$ .

So you see again here that it is not necessary that the gradient of the temperature should be 0. So long it satisfied this inequality that we have shown here that is sufficient for the drift diffusion model.

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**Drift -Diffusion (DD) Current Density Model**

$$\mathbf{J}_n \approx q\mathbf{D}_n(\mathbf{E}) \cdot \nabla_x \mathbf{n} + qn\mu_n(\mathbf{E}) \cdot \mathbf{E}$$
$$\mathbf{D}_n(\mathbf{E}) = (kT_n/q)\mu_n(\mathbf{E})$$
$$\mu_n(\mathbf{E}) = \frac{\mu_{n0}}{\sqrt{1+(E/E_{cr})^2}}$$

Low field mobility

Summary of approximations

- Quasi-static approximation of  $J_n$  and  $W_n$
- Spatially quasi-uniform approximation of  $W_n$ ,  $F_W$  and  $T_n$
- $W_{n,thermal} \gg W_{n,drift}$

So here is a summary of this model. The equations for current density has only 2 terms diffusion and drift. You have an expression relating the diffusion coefficient to the mobility both are dependent on the electric field and the electric field dependence of mobility is given by this formula where the mu suffix N0 is called low field mobility. Summary of approximations are quasi-static approximations of the current density and kinetic energy density, spatially quasi uniform approximation of the kinetic energy density.

The kinetic energy flux and the carrier temperature, electron temperature and finally the thermal kinetic energy is much greater than the drift kinetic energy.

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**Drift -Diffusion (DD) Current Density Model**

$$\mathbf{J}_n \approx q\mathbf{D}_n(\mathbf{E}) \cdot \nabla_x \mathbf{n} + qn\mu_n(\mathbf{E}) \cdot \mathbf{E}$$
$$\mathbf{D}_n(\mathbf{E}) = (kT_n/q)\mu_n(\mathbf{E})$$
$$\mu_n(\mathbf{E}) = \frac{\mu_{n0}}{\sqrt{1+(E/E_{cr})^2}}$$

Low field mobility

- This equation is not as rigorous and of the same status as CB / continuity equation or Maxwell's equations, due to the many approximations involved.
- However, it is valid even for high  $E$  within the approximation limits.

Now as you see this equation is not as rigorous and of the same status as carrier balance or

continuity equation or Maxwell equations due to the many approximations involved. So we have made so many approximations and therefore this drift diffusion model is not of the same status as the carrier balance equation. If you note the carrier balance equation was derived from Boltzmann's Transport Equation and we made no approximations.

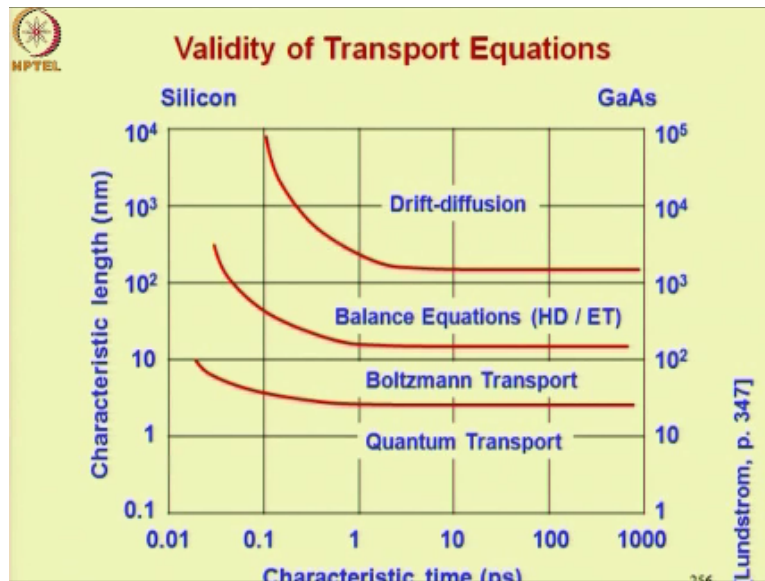
The equation is used as it is. However, there is a silver lining that the drift diffusion model is valid even for high electric field within the approximations limits. So we did not assume that the drift diffusion model works only for the small electric field regime where the drift velocity is linearly related to the electric field. Let us look at a comparison of the various models.

So we recall that had said that while for modeling the effects of electromagnetic field there are standard equations namely the Maxwell equations and the Lorentz force equation whereas for modeling the carrier transport in a semiconductor there are hierarchy and various levels of equations and various forms of equations. This is because we said that the movement of an electron in a semiconductor is fairly complex.

The electron undergoes random thermal motion. It collides with so many particles which are present, so many entities which are present in a semiconductor and then there is a directed motion, super imposed over this random motion and millions of electrons and holes are all colliding with each other and moving and causing the flow of current. So because the situation is complex there are many ways of approaching the modeling of this problem.

And that is why the plethora of equations and levels of equations.

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So it will be useful to look at these equations and see their validity range that is what is shown here. Now let us consider some samples to understand this figure. Now what you find on the Y axis is the characteristic length. This can be regarded as for example the length of the device. Now on the one side left hand side you have the lengths corresponding to silicon. And on the right hand side you have the lengths corresponding to Gallium arsenide.

The X axis is the characteristic time. So you see to decide the range of validity of the model we need to consider the device size and the time varying nature of this signal at what rate is the signal varying. Based on these 2 factors you can decide which range of models can be used. Note that the characteristic length of silicon is smaller than that of Gallium arsenide. What is the reason?

The reason for this is that the effective mass of electrons in Gallium arsenide is much smaller than that of silicon. So what implications does it have? So it has the following implications. For example, you take a Gallium arsenide device of 1-micron size. You see that no matter what is your frequency range. So here the frequency range would be say 1000 picoseconds characteristic time would mean 1 gigahertz.

So these are higher than 1 gigahertz. So over the frequency range considered here a 1-micron size Gallium arsenide device you have to use the energy balance equation you cannot work with drift diffusion. Note that in this drift diffusion model we have considered the velocity saturation effects also. So we are looking at a drift diffusion model with field dependent mobility.

So really speaking these balance equation regime is being used for modeling phenomena such as velocity overshoot. So what we find is that even a 1-micron Gallium arsenide device can exhibit velocity overshoot effects and so on and therefore you will have to use energy balance equation for modeling Gallium arsenide devices. On the other hand, the 1-micron silicon device falls well within the drift diffusion limits so long as your frequency is less than thousands gigahertz.


So this is 1000 gigahertz. Now that is fairly high frequency so you can model silicon devices to fairly high frequencies. However, model silicon devices are becoming smaller and smaller. So they will show velocity overshoot effects. So while 1-microns silicon device MOSFET for example may not show velocity overshoot effects when you are operating at the normal frequency ranges some micron device point 1-micron silicon device however will show velocity overshoot effects.

And therefore the balance equations will have to be used for modeling this. So when do we enter the Boltzmann's Transport regime really if the 3 balance equations are not sufficient to model the phenomena and we need more balance equations then instead of using more balance equations we go into the direct solution of the Boltzmann's Transport Equation and if the device size is further very small so nanoscale devices for example.

So you may have to go to quantum transport. Similarly, for high frequencies also you cannot use for example the drift diffusion model. Here you can see that around this region you are not able to use the drift diffusion model. However, these frequencies are really very high. So we will have opportunity to look at this figure once more when we discuss the characteristics times and lengths.

And see how based on characteristics time and length values we can use this figure and arrive at some conclusions regarding which model is to be used under what situation.

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## Extending the DD Model into the Balance Equation Regime

Aware of its approximate status, the DD equation has allowed empirical corrections to itself to extend its validity, and has been rather successful in this attempt, e.g., velocity overshoot can be modeled by adding terms as below.

$$J_n \approx qn \left[ \mu_n(E)E + W(E)\partial_x E + B(E)\partial_t E \right] + qD_n\partial_x n + A(E)\partial_t n$$

Corrects for  
spatial velocity  
overshoot

Corrects for  
Transient velocity  
overshoot

Preserves  
invariance of  
total current

[Thorner (1982) IEEE EDL, p. 69]

Now extending the drift diffusion model into the balance equation regime aware of its approximate status the drift diffusion equation has allowed empirical corrections to itself to extend its validity and has been rather successful in this attempt. So while the negative feature of the drift diffusion model is that lot of approximations have been made.

The positive side is since anyway so many approximations have been made one tries to treat this equation more and more to see whether you can model for example velocity overshoot by using empirical constant. So that is the kind of things that you can do with drift diffusion model. So because already it is very approximate so why not subject it to some further modifications if you can get some advantage out of it.

So for example velocity overshoot can be modeled by adding terms such as here is an example. So this is a drift diffusion equation. The terms in black color are the terms of the drift diffusion equation and the terms in blue you can see that 3 terms have been added. These are the ones which have been added to model velocity overshoot. Now there is a term dependent on this spatial gradient of the electric field.

There is a term dependent on the time variation of the electric field and there is a term involving the time variation of the carrier concentration. So this way you see that you are trying to complete the picture by adding time varying and spatially varying electric field terms and time varying and spatially varying concentration terms. So you are retaining all this kinds of variation in the equation hoping to model velocity overshoot.

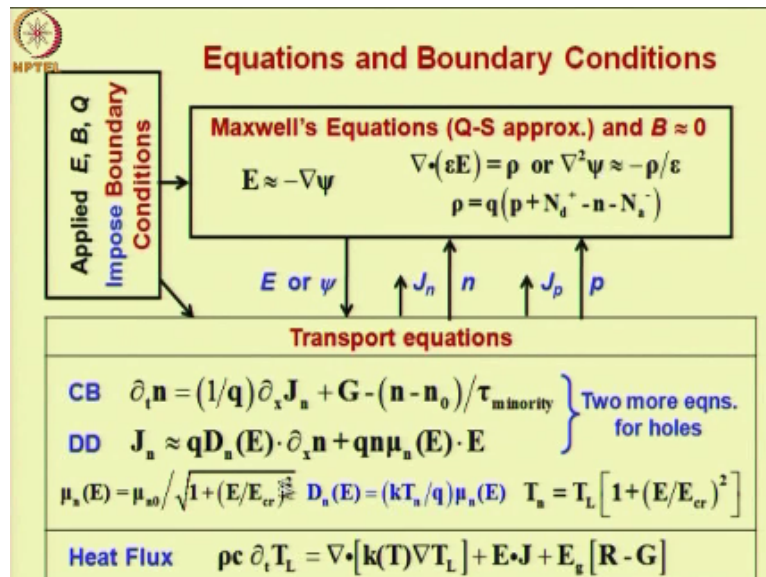


So you know that velocity overshoot results if the electric field suddenly changes as a function of distance or time. Therefore, the  $J_n$  current has been made dependent on these 2 terms. So the term involving the spatial gradient of the electric fields correct for spatial velocity overshoot. The term involving time variation of the electric field corrects for transient velocity overshoot.

And this term which depends on time variation of the carrier concentration it preserves the invariance of total current. So you recall we discuss that even when the velocity overshoot is there the total current from one contact to the other contact remains constant if there is no generation or recombination. Now this fact also has to be borne in mind that is why you found that spatial velocity overshoot not only the velocity varies with distance.

The carrier concentration also varies with distance. So those kinds of things also should be modeled and that is why these terms the carrier concentration term also has been included. So even when the velocity varies with time there also the current should remain constant and therefore this time varying time here of concentration.

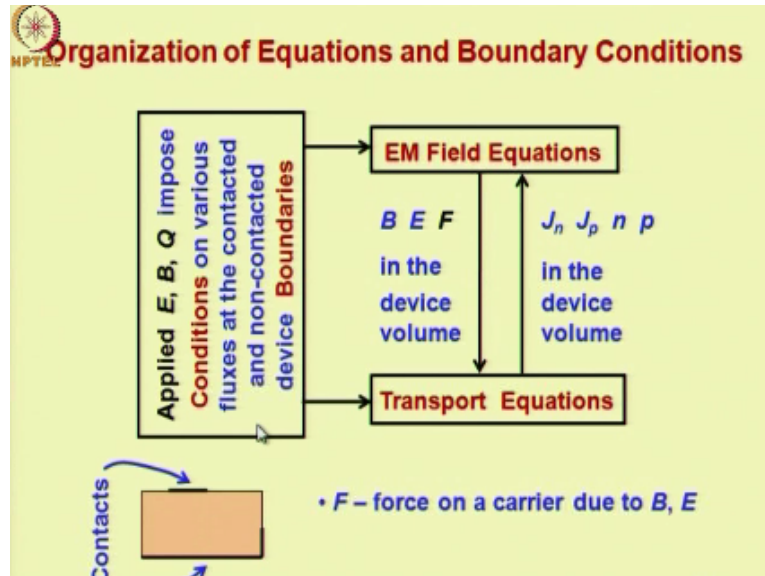
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So we can summarize our drift diffusion model along the same lines that we did with the drift diffusion thermoelectric current model. Here again you have 2 equations for electrons and another 2 equations for holes. So you are absorbing the energy balance information in the electron temperature and field dependent mobility. Now with that we have completed a discussion of this module on equations for semi classical carrier transport.

Now since we discussed a large number of ideas a large number of equations it would be useful to go through the various concepts and equations that we discussed once. Now that is what we will do towards the end of this module.

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Let us begin with the organization of equations and boundary conditions. So we said the equations and boundary conditions organizations are as follows. You have a set of electromagnetic field equations which give you information about the magnetic field, the electric field and the force due to electric and magnetic field. This information is used by the transport equation to give you information about the current density of electrons.

Current density of holes electron concentration and hole concentration and information about this current densities and carrier concentration is acquired by the electromagnetic field equations to give you the information about BE and F. Now that is why these 2 sets of equations the electromagnetic field equations and transport equation are coupled to each other. To solve these equations, you need the boundary conditions.

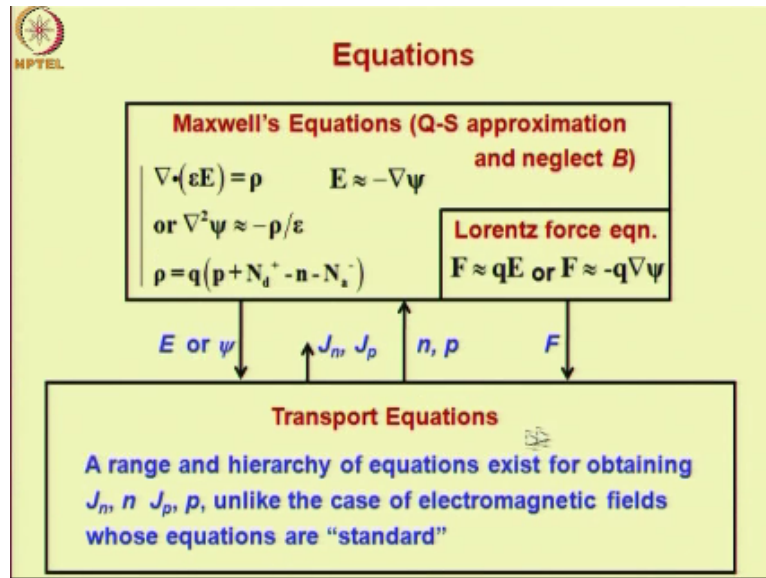
So the applied electric field magnetic flux and heat flux impose conditions on the various fluxes at the contacted and non contacted device boundaries. So here is an example showing the various boundaries. So you have one contact here and other contact at this end and you have the remaining boundary as non-contacted boundary. Now what we did was we entered into each of these boxes and then discussed the equations.

We did not pay much attention to the boundary conditions at this point. This is something that

we will do when we discuss the drift diffusion model in detail giving the complete expression for mobility including all scattering effects, generation recombination terms and so on. So at that point we will discuss the boundary conditions because that is the model that we are going to use in this course.

And actually solve current versus voltage characteristics for devices using the model.

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Let us enter into the electromagnetic field equations. So we gave the 4 Maxwell equations. This is equations for space charge used in the Gauss's Law and this is the Lorentz force equation. Now the  $J_n$  and  $J_p$  this arrow should actually be shown right up to this point because the  $J_n$  and  $J_p$  is required to get the curl of the magnetic field here. So this arrow should really be shown up to this point.

Now most often we use quasi-static approximation and neglect the magnetic fields. Under these conditions the 4 Maxwell equations reduce to just 2 equations. One is the equation for electric field in terms of the scalar potential and the other one is Gauss's Law in which if you substitute the equation for electric field in terms of scalar potential you get the Poisson's equation.

Now in deriving this equation we have assume that the epsilon or dielectric constant is not dependent on space. So it is spatially uniform and the Lorentz Force equation reduces to a simple formula  $F = Q$  times  $E$  assuming a positive charge  $Q$  or  $F = -Q$  times gradient of potential. Now with this approximation your  $J_n$  and  $J_p$  here are no more required to solve the

Maxwell equations that is a considerable simplification.

So the coupling points reduced. So now you have only 3 points of coupling namely the electric field or potential or carrier concentration of electrons and holes. The force on the electron is depended on the electric field itself. So really this is not an additional point of coupling. Now let us look at the transport equation a range on hierarchy of equations exist for obtaining  $J_n$   $N$   $J_p$  and  $P$  unlike the case of electromagnetic fields whose equations are standard.

So you have equations which yield you this quantity.

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The slide is titled "General Form of Transport Equations" and features the NPTEL logo in the top left corner. Below the title, it states "Each transport eqn. expresses conservation of some quantity". The main content is a physical interpretation of the continuity equation, presented as follows:

Physically

Rate of quantity increase in a small volume at $x$	=	Net influx of quantity into the volume	+	Net rate of quantity increase within the volume due to G-R processes
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Below this text, the mathematical equation is shown with arrows pointing from the text above to the corresponding terms in the equation:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \left( \frac{\mathbf{J}_p}{q} \right) + G_p - R_p$$

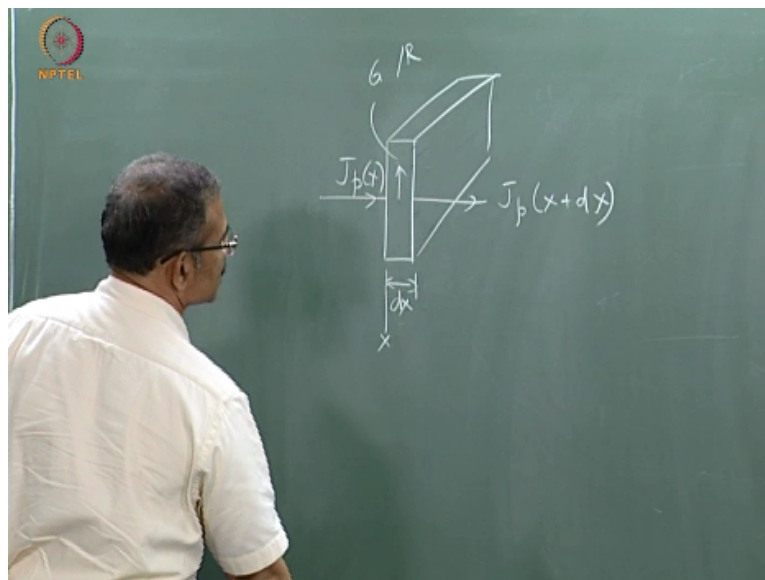
Now we discuss the general form of transport equations. We said that each transport equation expresses conservation of some quantity. Now this is very important because once we recognize that equations have some common form we feel very comfortable with them and we do not find difficult to remember these equations. And more than that in a new situation if we are asked to write equation for some quantity that is new kind of conservation equation we can immediately write out a form of this equation.

So that is the advantage of knowing the form. So general form we said can be regarded as similar to the whole continuity equation. So physically speaking the various terms of this equation represents what is shown here. The rate of quantity increase in a small volume at  $X$  is a left hand side this is equal to the net influx of quantity into the volume plus the net rate of quantity increase within the volume due to generation recombination process.

Now it is important to note that this equation set out in words needs a small manipulation to bring it in the form shown here. So when it is written in this form this equivalent to multiplying  $\frac{dP}{dt}$  with the volume. So this multiplied form product form in which the  $\frac{dP}{dt}$  is multiplied by volume is what comes here and similarly this term also multiplied by the volume term will come here.

So instead of talking about concentration which is what this equation talks about here we are talking in terms of the number in the entire volume rather than the concentration that is the only difference. So this statement of equation in words is obtained by multiplying each of the terms of the equation shown here by the volume.

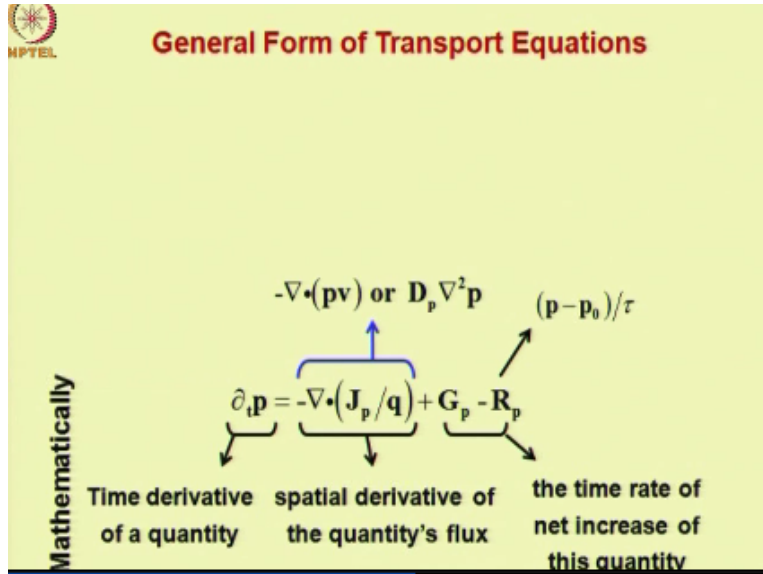
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So the continuity equation is about rate of change taking place in a volume like this. So this is the input, this is the  $DX$  at any  $X$  and this is the input this is the output. So difference of these 2 is the net input and inside there can be some generation or recombination. So that is represented by the terms  $G$  or  $R$  and because of the net input and because of  $G$  and  $R$  the carrier concentration inside can go on increasing or the number of carriers can go on increasing.

So whatever we have stated in words refers to the number of carriers within this volume that is shown whereas the equation itself talks in terms of the concentration of carriers.

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Now in mathematical terms which will be very useful for us the equation has following form the time derivative of a quantity is equal to the negative sign and spatial derivative of the quantity is flux plus the time rate of net increase of this quantity so these are called source terms. Now we said that this spatial derivative of the quantity is flux can be expressed in 2 alternate forms.

So the flux itself can be expressed either as a quantity for which we are adding the equation multiplied by the velocity or if you assume the flux of the quantity to depend on the quantity is spatial gradient like in diffusion then this diversion term comes out in the form delta square of the quantity multiplied by constant. So both these forms are possible for this term. Now depending on which form makes physical sense in a given situation we chose the particular form.

We will see shortly with all the examples. Similarly, the recombination due to electron hole pair recombination the loss in holes because of electron hole pair recombination is represented as the deviation of the hole concentration from the equilibrium multiplied by 1/tau. So constant into the quantity that is what is the form. So this form also is useful to note because in many physical situations we will find this form is being used.

So let us now just summarize all the equations and show how they can be cast in the form of this equation.

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**General Form of Transport Equations**

$$j\hbar\partial_t\psi(\mathbf{r},t) = -\left(\frac{\hbar^2}{2m_0}\right)\nabla^2\psi(\mathbf{r},t) + U(\mathbf{r},t)\psi(\mathbf{r},t)$$

$$\rho c \partial_t T_L = \nabla \cdot [k(T)\nabla T_L] + E \cdot J + \epsilon_g [R - G]$$

**Mathematically**

$$\partial_t p = -\nabla \cdot \left( \frac{J_p}{q} \right) + G_p - R_p$$

$D_p \nabla^2 p$   
 $\frac{1}{\tau}(p - p_0)$

Time derivative of a quantity    spatial derivative of the quantity's flux    the time rate of net increase of this quantity

So let us look at Schrodinger equation and the equation for heat flux. Now the corresponding terms are represented in the same color. So let us take Schrodinger equation. The quantity here is the wave function psi. So you have a time derivative of this quantity on the left hand side. Now you do have some other constants this can always be shifted to the right hand side that is not a big issue.

Similarly, here you have delta square of the wave function. This is analogous to delta square of the hole concentration. If you assume that flux of holes due to diffusion. Similarly, here you have the wave function multiplied by the term this happens to be potential energy term. So this is the source term much the same way as you use the term here. Though it is used as a sink so it is only a matter of sign source and sink.

So this kind of term you have here. We have also explained that how the other coefficient in this equation arise. So we said that the psi is a complex quantity in both X and T and therefore when you differentiate it with respect to X you get a J out and you differentiate twice with respect to X you get the twice of J out. So J into J and that is why you have a negative sign here.

On the other hand, when you differentiate it once with respect to time you have one J term out so that is what explains how this J is here. Similarly, since the coefficient here is a potential energy you can interpret the right hand side terms as kinetic energy + potential energy and accordingly you can arrive at H cross square/2 M 0 term and then for dimensional consistency you have H cross term coming here.

Now similarly the equation of lattice heat flux. You have time derivative of the lattice heat the left hand side. You have spatial derivative, spatial diversions derivative of the flux of this temperature that is the heat flux which is written in the form of the diffusion current of holes that is the heat flux is regarded proportional to the gradient of the lattice temperature gradient of the quantity. When you have the source terms here.

So these source terms are analogous to the net source terms here.

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**General Form of Transport Equations**

$$\partial_t f = -\nabla_r \cdot (f v) - \nabla_p \cdot (f F) + \partial_t f|_{\text{coll}} + s$$

$$d_t p = -\nabla U(r, t)$$

**Mathematically**

$$\partial_t p = -\nabla \cdot (J_p / q) + G_p - R_p$$

$-\nabla \cdot (pv)$   
 $\partial_t p|_{G-R}$

Time derivative of a quantity    spatial derivative of the quantity's flux    the time rate of net increase of this quantity

Now let us look at 2 more equations. The Boltzmann Transport Equation and the Newton's Law. The Boltzmann Transport Equation has time derivative of the distribution function so this is analogous to  $\frac{dP}{dT}$ . Then it has this spatial derivative of the flux. So  $F$  into  $V$  this analogous to  $P$  into  $V$  form a flux of the holes and there is a negative sign. Now while  $P$  here is a function of only  $R$  and  $T$  that is position and time.

The distribution function is a function of position momentum and time. And therefore you have 2 gradients here position and momentum gradients. So this is the momentum gradient term again with a negative sign analogous to the spatial gradient term and this is the flux if you replace the distance excess by the momentum excess. So  $\frac{DP}{DT}$  so velocity is  $\frac{DX}{DT}$  the velocity in the momentum excess is  $\frac{DP}{DT}$  that is force.

So that is how you get this term and then you have a source term  $\frac{dF}{dT}$  due to collisions. So this is momentum generation because of collision or loss. Now this is



analogous to this entire net excess generation term being cast as  $\frac{dP}{dT}$  or due to generation recombination. So if we use this Nomenclature use for Boltzmann Transport in the context of the hole continuity equation we could have written this term  $G_p - R_p$  as  $\frac{dP}{dT}$  corresponding to generation recombination.

Then you have another source term which takes into account this generation recombination that we have discussed. So while this is the generation or recombination or increase in loss of momentum, increase in loss of the distribution function due to momentum. This is the contribution of the electron hole pair generation recombination processes. Let us look at the Newton's Law.

So you have a time derivative of momentum on the left hand side and spatial gradient or derivative with a negative sign of the flux of this momentum. Now dimensionally this turns out to be the energy.

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**General Form of Transport Equations**

$$\partial_t n_\phi = -\nabla \cdot \mathbf{F}_\phi + G_\phi - R_\phi + S_\phi$$

$$\partial_t \mathbf{J}_n = (2q/m_n) \partial_x W_n + (q^2 E n / m_n) - (J_n / \tau_M)$$

$$\partial_t W_n = -\nabla \cdot \mathbf{F}_W + \mathbf{E} \cdot \mathbf{J}_n - (W_n - W_{n0}) / \tau_E + S_E$$

**Mathematically**

$$\partial_t p = -\nabla \cdot (\mathbf{J}_p / q) + G_p - R_p$$

$-\nabla \cdot (\mathbf{p}v)$   
 $\frac{1}{\tau} (p - p_0)$

Time derivative of a quantity  
 spatial derivative of the quantity's flux  
 the time rate of net increase of this quantity

The balance equation they are also of the same form as hole continuity equation. So  $\frac{dN_\phi}{dT}$  is same as  $\frac{dP}{dT}$ . Then you have negative divergences of the flux of  $N_\phi$  the same as negative divergences of the hole flux. Then you have several source and sinks terms here.  $G_\phi$  is the generation of  $N_\phi$  due to applied force and so on. So the term in Boltzmann transport equation which depends on the force works out as the generation term.

When you convert it into balance equation by summing over all the momentum states then you have a loss of  $N_\phi$  maybe because of things such as collision and then you have a

source term generation of the term  $N \phi$  because of electron hole pair generation recombination process. Now while this is general form when you want to write when you write this equation for momentum balance it works out in this form.

So we have discussed that the current contains the momentum term. So we can use the current density which is a vector as an equivalent of the momentum because we are actually interested in the current density rather than the momentum. So writing in terms of the current density the momentum balance equation has this form. So you have a time derivative of the current density on the left hand side analogous to  $\frac{dP}{dt}$ .

Then you have a spatial gradient of the flux of  $J_n$  which is the kinetic energy density term then you have the source term here. This is corresponding to  $G \phi$  term. You can see the field coming here. So this is the contribution to the current due to field. The  $R \phi$  term translates to  $J_n / \tau_M$  this is somewhat like this. So where you have a loss term proportional to the quantity proportionality constant being one by time constant.

This is exactly similar except that you do not have  $J_n$  suffix 0 like the  $P$  suffix 0 because while the hole concentration under equilibrium is non 0 the current density in equilibrium is 0 because in equilibrium you have random motion and there is no net flow in any direction. Now I would like to explain one point here that there is no  $S \phi$  term in the momentum balance equation. So we said the  $S \phi$  term is 0.

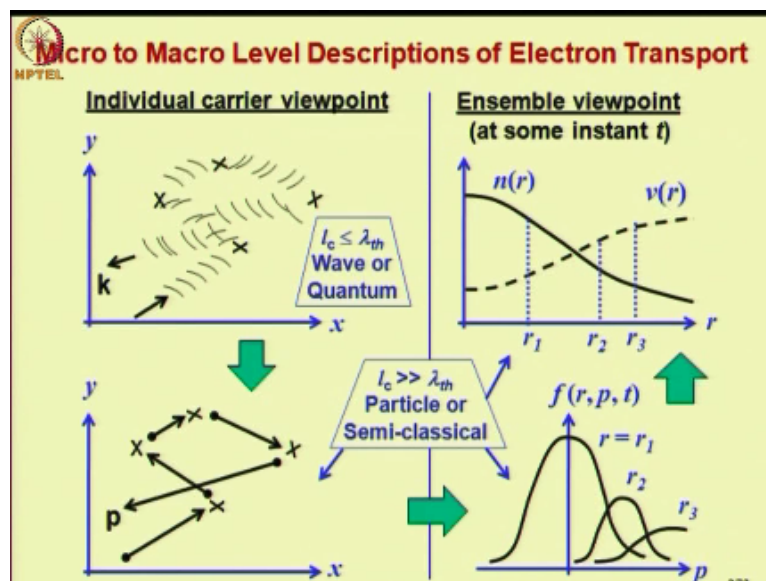
So why did we say  $S \phi$  is 0?  $S \phi$  is a source term because of electron hole pair generation some net generation of electron hole pairs. Now assuming here that all the electron hole pairs which are generated they have momentum in random directions. Therefore, together they do not contribute any net momentum or net current so that is why the  $S \phi$  term is said to 0. So they have momentum, the generated electron hole pairs have momentum random direction meaning they are in random motion.

After they are generated there is no preferred direction in which they move. The energy balance equation time derivative of  $W_n$  analogous to time derivative of  $\frac{d}{dt}$  hole concentration then negative gradient of the flux of kinetic energy then you have  $E \cdot J_n$  as the source term corresponding to  $G \phi$  generation of kinetic energy because of electric fields. So this contributes to the heat and then you have a term corresponding to  $R \phi$  that is  $W_n$ -

$W_n$  by the energy relaxation time.

So this loss term loss in energy term is exactly analogous to  $P-P_0/\tau$ . So unlike in the case of momentum balance equation where  $J_n$  at equilibrium is 0 the  $W_n$  kinetic energy under equilibrium is non 0 that is why this form is perfectly analogous to this form. And then you have some source terms the source of kinetic energy because of carriers which are generated electron hole pairs which are generated or recombined.

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Now let us look at the various descriptions of electron transport that we gave. So we discussed the 4 levels micro to macro level. The fundamental level is electron is a wave between 2 collisions. This level works when the mean free path or device size is less than the thermal average wave length or this thing works or we have to refer to this particular approach if really you have such small devices.

On the other hand, when the mean free path is much greater than the thermal average wave length we can use a particle approximation for the electron and you have 3 possible levels discussed here. The most fundamental level here is again individual carrier view point you treat every carrier individually at the particle between 2 collisions obeying Newton's laws. The next higher level is an Ensemble level where instead of using particles individually because there are millions of particles you look at them as a group.



And you talk in terms of the distribution function which talks about the distribution of a collection of electrons or momentum space and time. Very often this much detail information

about the distribution of electrons or momentum is not required and therefore you average out that information and instead you talk about an average carrier concentration as a function of position and time and average velocity as a function of position and time.

So the product of the carrier concentration and velocity and the charge, you know, gives you the device current.

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**Transport Equations – Individual Electron Viewpoint**

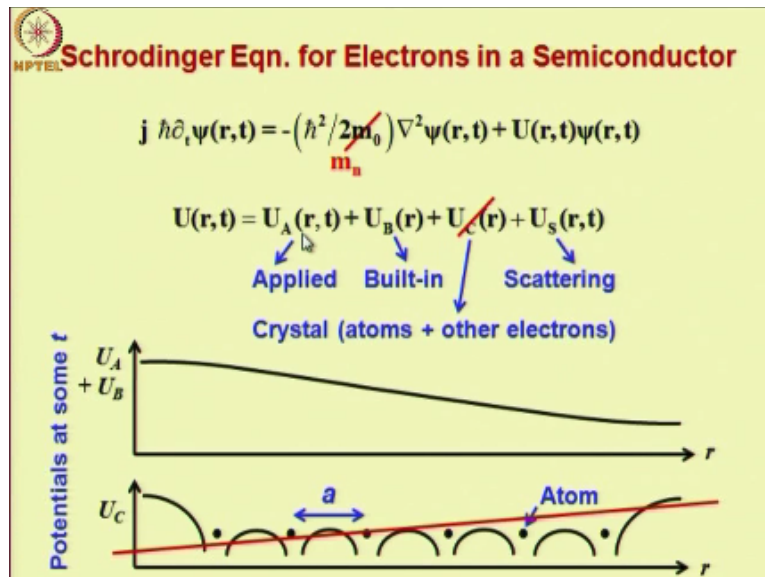
Viewpoint	Derivation of $n(r,t)$ and $J_n(r,t)$ due to $N$ electrons
<p>Carriers are waves</p> 	<ul style="list-style-type: none"> <li>Solve for the probability amplitude function <math>\psi_i(r, t)</math> from <u>Schrodinger equation</u>, where the crystal potential is ignored and <math>m_0</math> is replaced by <math>m_n</math></li> </ul> $n = \sum_{i=1}^N  \psi_i ^2 \quad J_n = -q \sum_{i=1}^N \frac{\hbar}{2m_n} \text{Im} [\bar{\psi}_i \nabla \psi_i - \psi_i \nabla \bar{\psi}_i]$
<p>Carriers are particles</p> 	<ul style="list-style-type: none"> <li>Solve for the position <math>r_i(t)</math> and momentum <math>p_i(t) = m_n v_i(t)</math> from <u>Newton's second law</u>.</li> <li>Identify <math>\delta N</math> e<sup>-</sup> having <math>r_i</math>'s in local volume <math>\delta V</math></li> </ul> $n = \frac{\delta N}{\delta V} \quad J_n = \frac{-q}{\delta V} \sum_{i=1}^{\delta N} \frac{p_i}{m_n}$

Now we discuss or rather outline the method of calculating current in each of the approaches. So for example if you regard the individual carrier viewpoint and take the carrier as waves then what do you do is you solve the probability amplitude function psi for each electron I from Schrodinger equation and if you ignore the crystal potential then replace the M 0 of Schrodinger equation by effective mass MN and then you use this formulae for finding out the current.

On the other hand, the analogously if you regard the carriers as particles and take the individual carrier viewpoint then for each particles you determine the state of the particle using Newton's Law. Now the state of the particle is nothing, but the position RIT for the I particles and the momentum PIT and you get it from Newton's second law.

Then you identify delta N electrons having their positions in local volumes delta V and from there you can derive the carrier concentration using this formula and the current density using the formula here.

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The Schrodinger equation for electrons when you use the wave approach is given here. The potential term when you are dealing with electron semi crystal consists of several components such as the applied potential, the built in potential, the crystal potential which consists of the effects of atomic nuclei and other electrons and holes and the scattering potential which is a random potential.

Now what is interesting to note is that the crystal potential varies very rapidly over small length scale of the lattice constant  $A$ . Whereas the applied and built in potential very rather slowly. It is this difference in the variation of the components that allows you to use the effective mass approximation. So we said that because the crystal potential varies. So rapidly over length scale  $A$  which are very small compared to the thermal average De Broglie wave length of the carrier or electrons.

We have to refer to solution of Schrodinger equation to model this effect and this is what we do by doing the effective mass. On the other hand, once you use the effective mass concept then the effect of this potential can be treated using Newton's law. So when you remove the crystal potential or absorb it effects in the effective mass then  $M_0$  is change to  $M_N$  and your solution then has to only take into account the potential  $U_A$ ,  $U_B$  and the scattering potentials.

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**Newton's 2<sup>nd</sup> Law for Electrons in a Semiconductor**

$$m_n^* \left( \frac{d^2 \mathbf{r}(t)}{dt^2} \right) = \mathbf{F}(\mathbf{r}, t)$$

$$\mathbf{F}(\mathbf{r}, t) = -q \left[ \mathbf{E}_A(\mathbf{r}, t) + \mathbf{E}_B(\mathbf{r}, t) + \mathbf{E}_C(\mathbf{r}, t) \right] + \mathbf{F}_S(\mathbf{r}, t)$$

Applied Built-in Scattering  
Crystal (atoms + other electrons)

Analogously, if you use Newton second law and use the particle approach then this is the equation of Newton second law. And just analogous to all the potential terms you have the force terms. So applied electric field, the built in electric field, the crystal electric field because of atoms and other electrons and this scattering forces.

So we remark that while the quantum mechanics uses gradient of potential energy while the quantum mechanics uses potential energy for action. The classical mechanics or Newton's law uses gradient of potential energy or force. Now when you remove the crystal electric field then you replace MO/MN effect of crystal potential are absorbed in this effective mass.

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**Transport Equations – Ensemble Viewpoint**

For carrier population  $N \gg 1$ , the carriers are better treated collectively rather than individually

Viewpoint	$n(r,t)$ and $J_n(r,t)$ derived from
Carriers as ensemble of waves	quantum distribution function solved from Quantum Transport Equation (QTE)
Carriers as ensemble of particles	classical distribution function $f(r, p, t)$ solved from Boltzmann Transport Equation (BTE)

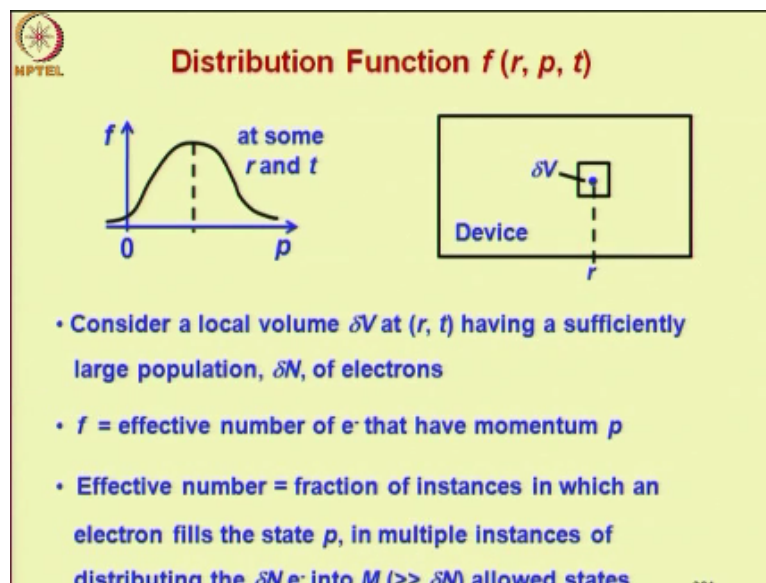
We adopt the particle ensemble viewpoint in this course

Now coming to transport equations the ensemble viewpoint when the carrier population is rather large then we treat the carrier collectively rather than individually you have 2

viewpoints either regard the electrons as ensemble of waves or ensemble of particles. If you regard as ensemble of waves when use the quantum transport equation to solve for the quantum distribution function and from that you get the carrier concentration and current density.

Now, if the carriers are regarded as ensemble of particles then use the Boltzmann Transport Equation to solve for the distribution function  $F$  and this is the approach that we have used in our course.

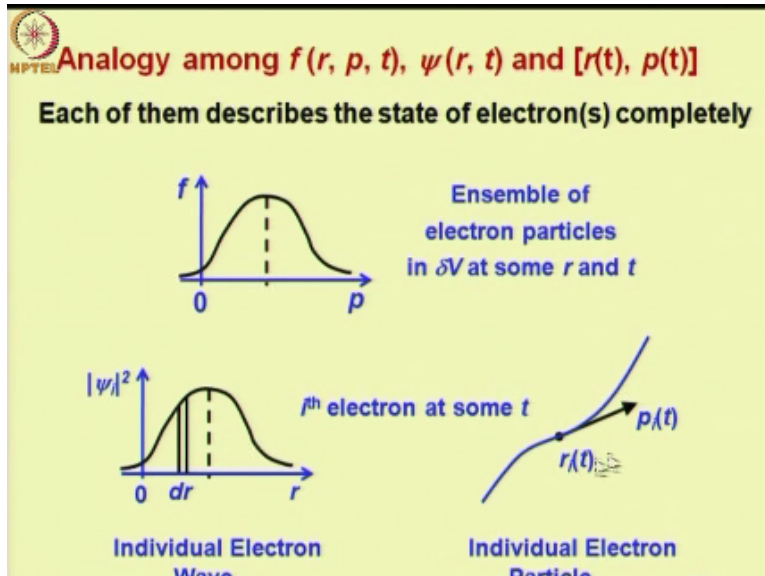
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The distribution function itself was discussed in great detail and explained. So to understand the distribution function consider a local volume  $\delta V$  at a position  $R$  at any instant  $T$  having a sufficiently large population  $\delta N$  of electrons. Now  $F$  is the effective number of electrons that have momentum  $P$  out of this population.

The effective number is nothing, but the fraction of instances in which an electron fills the state  $P$  or has a momentum  $P$  in multiple instances of distribution of  $\delta N$  electrons into the  $M$  allowed states.  $M$  is much greater than  $\delta N$ .

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Now we explained the analogy among the distribution function  $F$  the wave function  $\psi$  and the method of classical mechanics in which the state of a particle described in terms for the position and momentum combination. Now each of them described the state of electrons completely. So the distribution function describes the state of electrons as a state of an ensemble of electron particles in  $\Delta V$  at some position in time.

Interestingly, the wave function also has similar kind of shape and the area under the square of the wave function has the same meaning as the distribution function namely it gives the probability of finding the electron in this region. So similarly the individual electron particle is described in terms of the position  $R$  and momentum  $T$ .

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$$d_t f(\mathbf{x}, \mathbf{p}, t) = \partial_t f|_{\text{coll}} + s$$

$$\underbrace{\partial_t f + \overbrace{\partial_x f d_t x}^v + \partial_p f d_t p}^{\text{Classical Mechanics}} = \underbrace{\partial_t f|_{\text{coll}} + s}_{\text{Quantum Mechanics}}$$

$$\partial_t f = -v \partial_x f - F \partial_p f + \partial_t f|_{\text{coll}} + s$$

3-D version

$$\partial_t f = -v \cdot \nabla_r f - F \cdot \nabla_p f + \partial_t f|_{\text{coll}} + s$$

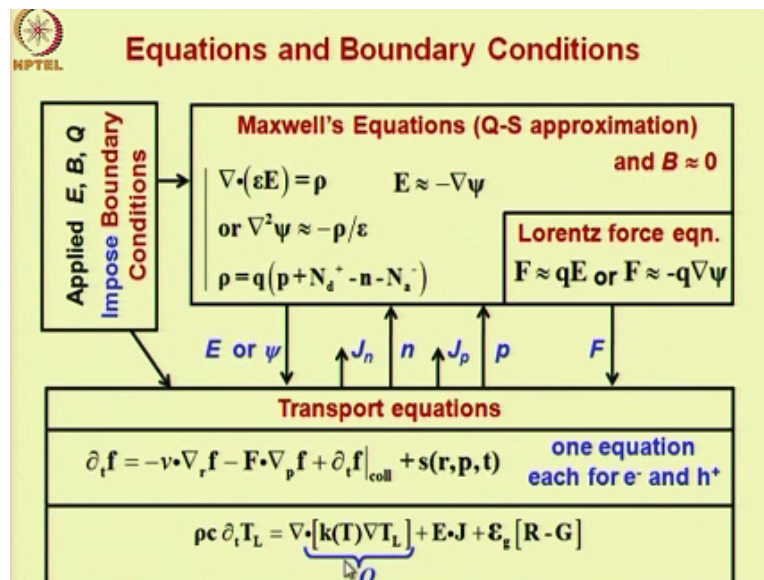
The Boltzmann Transport Equation in the most compact form it is  $DF/DT = \text{dout } F/\text{dout } T =$



collision + other source terms. Now the total differential D is because of various factors as you can see X, P and T are the 3 variables. So you expand then you get  $\frac{dF}{dT} + \frac{dF}{dX}$  into  $\frac{DX}{DT}$  which is nothing, but the velocity +  $\frac{dF}{dP}$  into  $\frac{DP}{DT}$  which is nothing but the force.

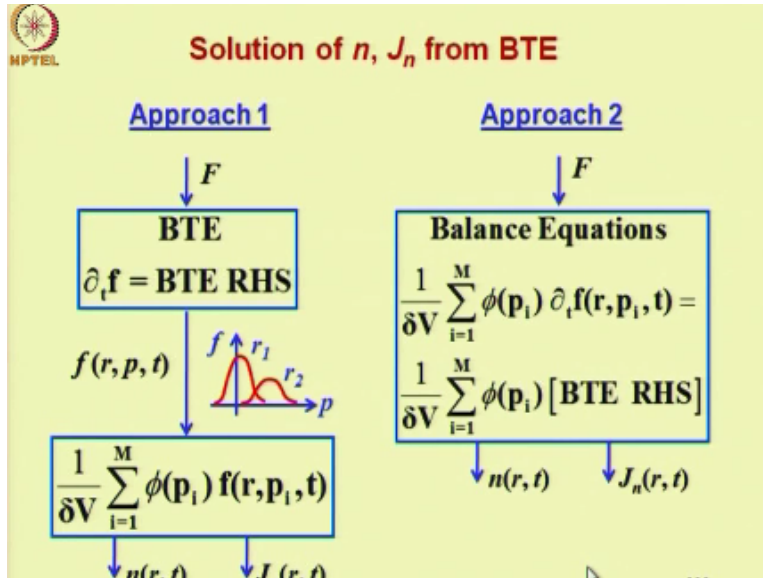
Now these 3 terms together represent the classical mechanics and the right hand side terms had to determine from quantum mechanics. So this is how the Boltzmann Transport Equation describes semi classical transport because it has both quantum mechanics and classical mechanics. In one dimensional form this equation was written like this and in the 3D version in this form.

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Now if you include the Boltzmann Transport Equation then your equations in boundary conditions picture looks like this. So you have one Boltzmann transport equation of electrons and another one for holes. And you need the heat flux equation also because the distribution function depends on the carrier temperature and if you want to solve the carrier temperature you need the lattice temperature and that is what is solved for using this equation.

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Now to derive the current density and carrier concentration from BTE we discussed 2 approaches. One approach you solve the BTE and get the distribution function then use this formulae to get the carrier concentration and current density. On the other hand, in the approach 2, you perform this operation on the distribution function in the Boltzmann Transport Equation itself.

And convert this equation into a set of balance equation for electron concentration, hole concentration, electron current, hole current then other terms like electron kinetic energy, hole kinetic energy and so on. And directly you solve for the carrier concentration and current density.

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Now you can estimate in the approach one the current density and carrier concentration and

kinetic energy from these formulae.

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**Displaced-Maxwellian Approximation of  $f(r, p, t)$**

$$f(r, p, t) \approx \exp\left[\frac{\mathcal{E}_{in}(r, t) - \mathcal{E}_c(r, t)}{kT_n(r, t)}\right] \exp\left[\frac{-|p - m_n v_d(r, t)|^2}{2m_n kT_n(r, t)}\right]$$

at some  $r$  and  $t$

Equilibrium  $T_n = T_L$   
 Quasi-equilibrium  $T_n \approx T_L$   
 Non-equilibrium  $T_n > T_L$

$$n(r, t) = N_c \exp\left[\frac{\mathcal{E}_{in}(r, t) - \mathcal{E}_c(r, t)}{kT_n(r, t)}\right] \quad J_n(r, t) = -qn(r, t)v_d(r, t)$$

$$W_n(r, t) = \left(\frac{1}{2}m_n v_d^2(r, t) + \frac{3}{2}kT_n(r, t)\right)n(r, t)$$

While solution of the Boltzmann Transport Equation is rather difficult one uses a guess which is called the displaced Maxwellian approximation. Now this case is arrived at by modifying the equilibrium distribution function. And if displaced Maxwellian approximation is used you get these expressions for carrier concentration, current density and kinetic energy density applying the formulae of the previous slide.

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**Equations and Boundary Conditions**

Applied  $E, B, Q$   
 Impose Boundary Conditions

**Maxwell's Equations (Q-S approx.) and  $B \approx 0$**

$$E \approx -\nabla\psi \quad \nabla \cdot (\epsilon E) = \rho \quad \text{or} \quad \nabla^2 \psi \approx -\rho/\epsilon$$

$$\rho = q(p + N_d^+ - n - N_a^-)$$

$E$  or  $\psi$      $J_n$      $n$      $J_p$      $p$

**Transport equations**

CB	$\partial_t n = (1/q)\partial_x J_n + G - R$	$R = (n - n_0)/\tau_{minority}$	Three more eqns. for holes
MB	$\partial_t J_n = (2q/m_n)\partial_x W_n + (q^2 E n / m_n) - (J_n / \tau_M)$		
EB	$\partial_t W_n = -\partial_x F_W + E J_n - (W_n - W_{n0})/\tau_E + S_E$		
Heat Flux	$\rho c \partial_t T_L = \nabla \cdot [k(T)\nabla T_L] + E \cdot J + E_g [R - G]$		

Now if you use the balance equation approach second approach the equation scenario is something like this. So you have the carrier balance equation, momentum balance equation and energy balance equation you terminate after the series of balance equations at the end of this step. And this FW term here you use the phenomenological relation in case you have to

use this term.

But we showed that you really do not need the information about this term in many situations. So you have 3 equations for electrons and 3 equations for holes.

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**Implications of Physical Conditions on Transport Equations**

Steady State:  $\partial_t(\text{Quantity}) = 0$

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**CB**  $\cancel{\partial_t n} = (1/q)\partial_x J_n + G - R$

**MB**  $\cancel{\partial_t J_n} = (2q/m_n)\partial_x W_n + (q^2 E n/m_n) - (J_n/\tau_M)$

**EB**  $\cancel{\partial_t W_n} = -\partial_x F_W + E J_n - (W_n - W_{n0})/\tau_E + S_E$

**Heat Flux**  $\cancel{\rho c \partial_t T_L} = \nabla \cdot [k(T)\nabla T_L] + E \cdot J + E_x [R - G]$

Under conditions such as equilibrium, steady state and spatial uniform many terms of the balance equations drop out under equilibrium all the time derivatives go away. Spatial derivatives also go away and many other terms also drop out. So this really becomes very simple situation. Under steady state all the time derivatives go away. Spatially uniform conditions, the spatial derivatives fall off.

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**Drift Velocity-Field Model**

Diagram: A rectangular device with an electric field  $E$  pointing right. Electrons ( $e^-$ ) drift left, and holes ( $h^+$ ) drift right. Current  $I$  flows out of the left terminal, and voltage  $V$  is applied across the terminals.

Graph: Plot of drift velocity  $|v_d|$  (in  $10^7 \text{ cm s}^{-1}$ ) versus electric field  $E$  (in  $\text{V } \mu\text{m}^{-1}$ ) for Si at 300K. The solid line represents Electrons, and the dashed line represents Holes. Both show a non-linear relationship that saturates at higher fields.

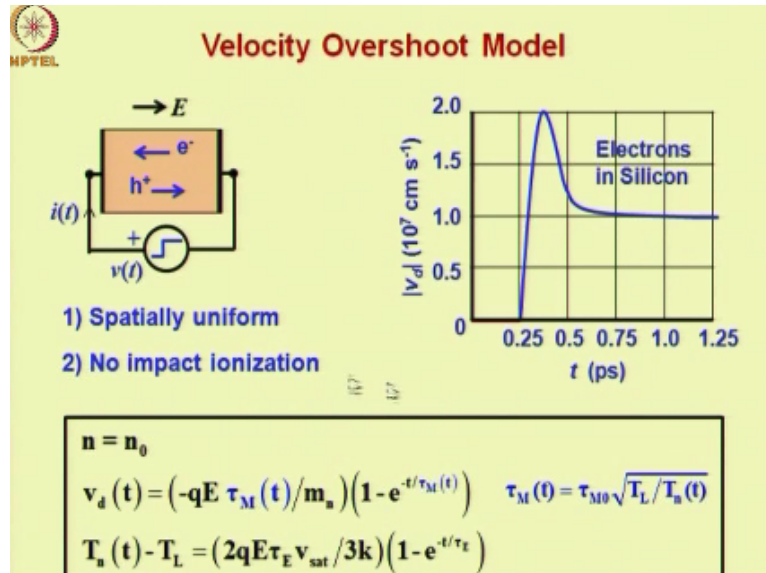
1) Steady state  
2) Spatially uniform  
3) No impact ionization

$$v_d(E) = \frac{-\mu_{n0} E}{\sqrt{1 + (E/E_{cr})^2}} \quad \mu_{n0} = \frac{q\tau_{M0}}{m_n} \quad v_{sat} = \lim_{E \rightarrow \infty} v_d = v_{th} \sqrt{\frac{\tau_{M0}}{6\tau_{E0}}}$$

Then we derive the drift velocity field model assuming steady state spatially uniform and no

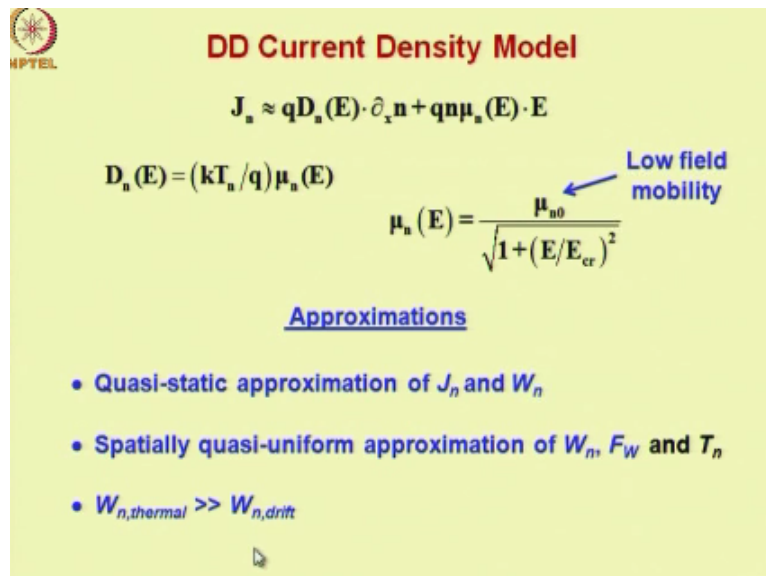
impact ionization conditions. We explained how the velocity saturation happens and saturation velocity depends on the thermal velocity and the velocity field curve shows a linear behavior for small electric fields.

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We also model the velocity overshoot assuming spatially uniform condition in the semiconductor and no impact ionization.

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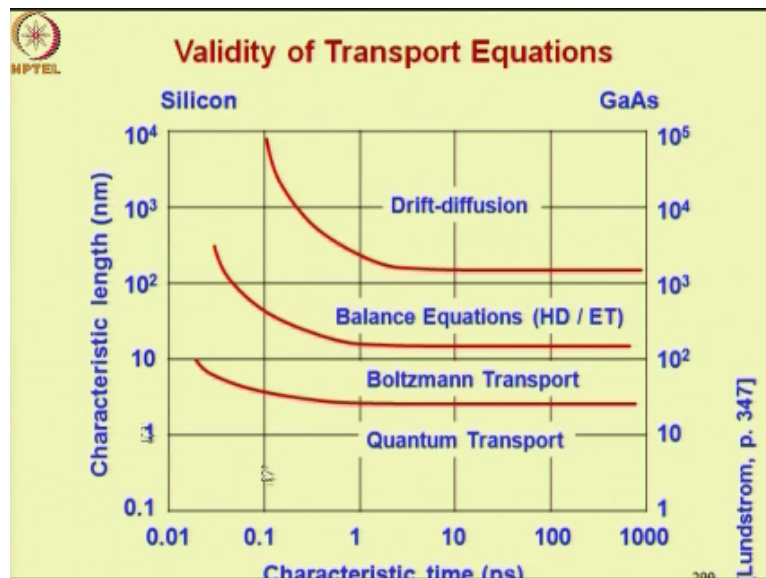
The drift diffusion thermoelectric current density model was given in terms of these equations and the approximations were that the quasi-static approximation of  $J_n$  and  $W_n$  the spatially quasi-uniform approximation of  $W_n$  and  $F_W$  and thermal energy much greater than the drift energy. The equations of drift diffusion and thermoelectric current have the form shown here.

So you have 2 equations for electrons and 2 equations for holes. This equation absorbs both effects of momentum balance as well as energy balance here the drift diffusion thermoelectric current equation. So as against energy balance case equations case there you had 6 equations 3 for electron, 3 for holes, you have 2 for electrons, 2 for holes. Apart from the heat flux equation.

The drift diffusion thermoelectric current equation can be further simplified to get the drift diffusion current density model. And the approximation here by quasi-static approximations for  $J_n$  and  $W_n$  spatially quasi-uniform approximation of  $W_n$ ,  $F_w$  and  $T_n$  and thermal energy much more than drift energy. Now this is how the drift diffusion model looks like and this is the model that we will be using throughout our course.


It has 2 equations for electrons, 2 equations for holes and an equation for the heat flux in the transport equations.

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We pointed out the validity of various regimes in terms of the time varying nature of the applied signal or the rate at which the applied signal varies with time and the device length for silicon and gallium arsenide.

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*Module 3*

### Semi-classical Bulk Transport: EM Field and Transport Equations


At the end of this module, you should be able to

- Write the equations of electromagnetic field driving the device current, namely -
  - Maxwell's wave equations and their quasi-static approximation
  - Lorentz force equation

300

So to summarize at the end of this module I hope that you are able to write the equations of electromagnetic field driving the device current namely Maxwell's wave equations and their quasi-static approximations, Lorentz force equation.

**(Refer Slide Time: 55:28)**



*Module 3*

### Semi-classical Bulk Transport: EM Field and Transport Equations


At the end of this module, you should be able to

- Recognize the four approaches of determining the device current, developed out of the individual carrier and ensemble viewpoints, in each of which the carrier can be treated either as a particle or as a wave

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Recognize the 4 approaches of determining the device current developed out of the individual carrier and ensemble viewpoints in each of which the carrier can be treated either as a particle or as a wave.

**(Refer Slide Time: 55:40)**



*Module 3*

**Semi-classical Bulk Transport:  
EM Field and Transport Equations**


At the end of this module, you should be able to

- Recognize that the equations of carrier transport in semiconductor devices have a common form which manifests conservation of some physical quantity

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Recognize that the equations of carrier transport in semiconductor devices have a common form which manifests conservation of some physical quantity.

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*Module 3*

**Semi-classical Bulk Transport:  
EM Field and Transport Equations**

At the end of this module, you should be able to


- Write the fundamental equations of determining the device current based on each of the following:  
Schrodinger equation, Newton's second law and Boltzmann Transport Equation (BTE)

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Write the fundamental equations of determining the device current based on each of the following namely Schrodinger equations, Newton second law and Boltzmann Transport Equation.

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*Module 3*


**Semi-classical Bulk Transport:  
EM Field and Transport Equations**

At the end of this module, you should be able to

- Write the equation for lattice temperature or heat flux, and recognize its necessity for determining the device current from the ensemble point of view

Write the equation for lattice temperature or heat flux and recognize its necessity for determining the device current from the ensemble point of view.

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*Module 3*

**Semi-classical Bulk Transport:  
EM Field and Transport Equations**

At the end of this module, you should be able to

- Derive the approximations of the BTE, namely:
  - carrier, momentum and energy balance equations
  - drift-diffusion and thermoelectric current equation
- Apply the balance equations to derive expressions for the velocity-field and velocity overshoot characteristics

Derive the approximations of the Boltzmann Transport equation namely the carrier, momentum and energy balance equations and drift diffusion and thermoelectric current equation and finally apply the balance equations to derive expressions for velocity field and velocity overshoot characteristics. Now with that we come to the end of this module. We will discuss the drift diffusion model in great detail in the next module.