

Semiconductor Device Modeling
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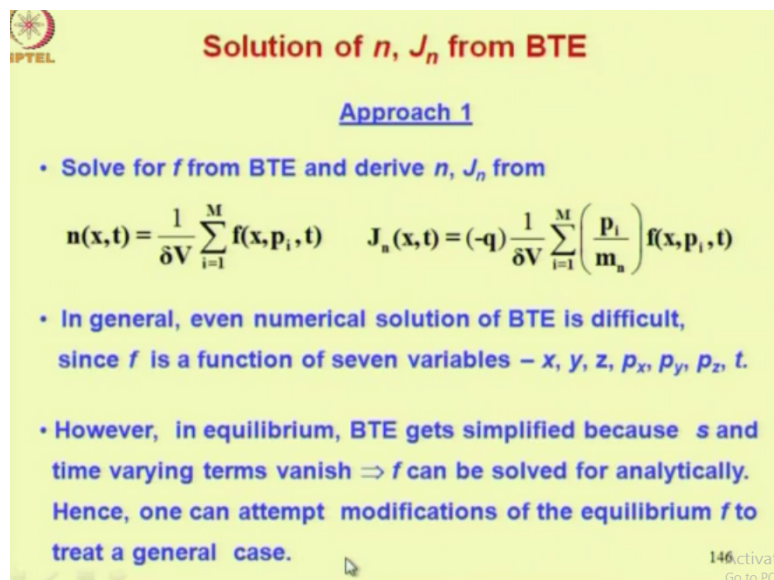
Lecture - 12
Semi-classical Bulk Transport: EM Field and Transport Equations

In the previous lecture, we began a discussion of the fundamental ensemble view point of getting the device current from a description of carrier population over momentum assuming the carriers are particles. So we explained in detail, what is the meaning of the distribution function and then we gave the formula for deriving n , J_n and kinetic energy density W_n from the distribution function f .

We also explained the equation which helps you to derive the distribution function F and that equation is called the Boltzmann's Transport Equation. We showed that this equation has close correspondence to the whole continuity equation. Therefore, it can be regarded as a balance conservation or continuity equation for the distribution function.

In this lecture, let us look at ways of solving the distribution function or ways of solving the Boltzmann's Transport Equation or working with the Boltzmann's Transport Equation to get the device current carrier concentration and so on. The first approach, you can solve for n and J_n as follows;

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Solution of n , J_n from BTE

Approach 1

- Solve for f from BTE and derive n , J_n from

$$n(x, t) = \frac{1}{\delta V} \sum_{i=1}^M f(x, p_i, t) \quad J_n(x, t) = (-q) \frac{1}{\delta V} \sum_{i=1}^M \left(\frac{p_i}{m_n} \right) f(x, p_i, t)$$

- In general, even numerical solution of BTE is difficult, since f is a function of seven variables – x , y , z , p_x , p_y , p_z , t .
- However, in equilibrium, BTE gets simplified because s and time varying terms vanish $\Rightarrow f$ can be solved for analytically. Hence, one can attempt modifications of the equilibrium f to treat a general case.

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You solve for the function f from the Boltzmann's Transport Equation and derive n and J_n from this formula which we wrote down in the first level course, which we wrote down in yesterday's lecture. Now, in general even numerical solution of Boltzmann's Transport Equation is rather difficult because f is a function of 7 variables. x, y, z, P_x, P_y, P_z and t .

So when you look at a picture in 3 dimensions then you see the distribution function really becomes complicated you are having 7 variables. If you look at in 1-dimension then you have only x and the P_x apart from t . But in 3 dimensions it is complicated. However, in equilibrium the Boltzmann's Transport Equation gets simplified because the term S and time varying terms vanish and so f can be solved for analytically. So, what we are saying is the following.

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BTE under equilibrium

$$\frac{\partial f}{\partial t} = -v \frac{\partial f_0}{\partial x} - F \frac{\partial f_0}{\partial p} + \frac{\partial f}{\partial x} \left(\frac{1}{\tau} \right) + \dots$$

$$f_0 = \frac{1}{1 + \exp\left(\frac{\epsilon + \frac{p^2}{2m_n} - \epsilon_f}{kT_L}\right)} = \frac{1}{1 + e^y}$$

$$f \frac{\partial f_0}{\partial y} \frac{dy}{dx} + f \frac{\partial f_0}{\partial p} \frac{dp}{dx} = 0$$

$$\frac{dy}{dx} = \frac{1}{kT_L} \left(\frac{d\epsilon}{dx} - \frac{d\epsilon_f}{dx} \right) + \frac{1}{k} \left(\frac{\epsilon + \frac{p^2}{2m_n} - \epsilon_f}{kT_L} \right) \frac{d}{dx} \left(\frac{1}{T_L} \right)$$

If you look at the equilibrium state then this Boltzmann's Transport Equation, which we write as follows. This term will be 0 because things will not change with time. This term will be 0 for the same reason things do not change with time and this term is also 0 because there is no excess generation or recombination. So, you see they are left with only these 2 terms = 0.

So this what we mean by saying on equilibrium the equation simplifies. So, can we now use this feature in some way? We will discuss analytical solution shortly, but before that let us make a point since the equilibrium solution is possible, analytically. Hence, one can attempt modifications of the equilibrium function f to treat a general case. So, we get a distribution function for equilibrium.

And for non-equilibrium cases what we do is we disturb this function or we pert up this function or modify this function by introducing some additional terms to represent the effect of non-equilibrium and we try to see whether this form satisfies the Boltzmann's Transport Equation. If so, then we regard this as the solution.

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The slide features a graph of a bell-shaped curve representing the equilibrium distribution function f as a function of momentum p . The curve is centered at $p=0$ and is symmetric. Below the graph, the equilibrium distribution function is given by the Fermi-Dirac distribution:

$$f_0(x,p) = \frac{1}{1 + \exp\left[\frac{\mathcal{E}(x,p) - \mathcal{E}_f}{kT_L}\right]}$$

The energy $\mathcal{E}(x,p)$ is expressed as the sum of the conduction band energy $\mathcal{E}_c(x)$ and the kinetic energy of the electron:

$$\mathcal{E}(x,p) = \mathcal{E}_c(x) + \frac{|p|^2}{2m_n}$$

Below these equations, it is stated that this form is a solution to the Boltzmann Transport Equation (BTE) under the following conditions:

$$\nabla_x \mathcal{E}_f = 0 \quad \nabla_x T_L = 0$$

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Let us look at the equilibrium solution for f . Let us attempt to check whether a form like this can work. Now this is really good guess work or imagination, right. Right now we cannot justify this form unless we show that it will satisfy the Boltzmann's Transport Equation and we also derive under what conditions it satisfies the Boltzmann's Transport Equation. Let us say, we have done an inspired guess.

Note that I have put a suffix 0 here to show that this is equilibrium situation and the t therefore has gone out of this set of variables. Let me read this thing for you, so f not affects, p which were trying as a solution has a form $1/1 + \text{exponential of } E$, the energy of the electron or energy of the state. At any x and it is a function of the momentum p - a constant level as we will see this is from E level.

Right now let us say it is some constant divided by K times T_L where T_L is the lattice temperature. Now, what is our motivation for thinking about a form like this, we will see that shortly. Mainly we would like to connect it to the shape of this function that we anticipate. So, we are looking at expression that will fit into this kind of a shape, okay for f as a function of P .

Now, the total energy E is nothing but the sum of potential energy which we represent as E_c . Now here please note that this is capital version of the Greek Letter Epsilon, however, we will simply continue to call it as E but you must always remember this is not the same as the symbol used for electric field. So, this is a potential energy of the electron. When we discuss the band structure, we will show that this energy nothing.

But the conduction band H in the energy band picture. That is the potential energy + the kinetic energy which is nothing by models of $P^2/2m_n$ where P is the momentum of the electron. So, this is the total energy potential + kinetic. Now we will show that this will be a solution of the Boltzmann's Transport Equation provided the gradient of Fermi level.

Well, probably we should right now avoid using the word Fermi level because right now we really do not know that this is a Fermi-Dirac distribution function, right? We are just guessing a form. So we pretend that we do not know. So, this constant E_f whatever we are using here the gradient of this special gradient of this should be zero in other words this constant should be same for all x on a 3 dimensions for all positions.

Similarly, the gradient of the lattice temperature should also be 0. In other words, lattice temperature should be uniform throughout the device. So, both E_f and lattice temperature should be constant throughout the device. So long as this is satisfied, so long as the constants here T_l and E_f follow this condition you can show that this function will be a solution of the Boltzmann's Transport Equation under equilibrium.

Now, let us do some manipulation to show that. This is our Boltzmann's Transport Equation, okay. Now, we will substitute this function f_0 and evaluate the derivatives which are there. Or rather derive the derivatives of this function. So, let us write this here. The form we are trying out is under equilibrium, this is f_0 . And the form we are trying out is $F = 1/1 + \exp(-(E - E_f)/kT_l)$ where this E is the total energy. So, let us write this total energy in terms of potential and kinetic.

So, this is $E_c + P^2/2m_n - E_f$. If this is the solution then when I substitute this in this equation the sum of the 2 terms should become zero. So, let us substitute and see what equations we get. So, we get V multiplied by now $\frac{df_0}{dx}$. Now, here this E_c is a

function X , okay? Now, E_f we can assume to be a function of x and later on get that it is not a function of x whatever.

Now this E_c is appearing in this exponential which is in the denominator. Now since this is a little bit involved what we can do is, we will make a substitution we will assume that this quantity is y then our f_0 turns out to be $= 1/1+e^y$. Now, it will be easy to work with that. Now, we use y as a variable then I can write $\frac{df_0}{dx}$ as $\frac{df_0}{dy}$ multiplied by $\frac{dy}{dx}$.

And similarly plus now I removing the negative signs, right $+f$, here also I do the same I write $\frac{df_0}{dy}$ multiplied by $\frac{dy}{dp}$. Sorry it is dy/dp and this is $= 0$. Now I can cancel out this $\frac{df_0}{dy}$. What is dy/dp ? So this is y . So, when I differentiate with respect to P , the E_c is not a function of P , it is a potential energy, right? It does not depend on momentum.

So derivative with respect to P of this quantity is 0. So, similarly E_f is also not a function of P . Therefore, what remains is only this, so if you take derivative of this with respect to P , I will get $2 \times \frac{P}{2Mn}$ which is $\frac{P}{Mn}$ and $\frac{P}{Mn}$ is nothing but the velocity, V which were using here. So, this dy/dp is velocity but there is a K times Tl in the denominator Tl is again not a function of T , you can treat as a constant.

So, this is V/K times Tl . Now if this is the case then this V also gets cancelled out of the equation. Now let us as look at dy/dx , so dy/dx . P is not a function of x , okay because x and P are independent variables. So, we have to take dE_c/dx and right now we do not know E_f could depend on x though it is not a function of P , we can assume E_f also to be depend on x and see what happens.

Thus the derivative Dy/dx would be now Tl also we should allow to be a function of x . Later on we can see that it will not be a function of x because of the imposition of the condition it should satisfy the equation. But since this is also a function of x , so I have numerator and denominator. So, basically a product of 2 terms, so I should be careful while looking at that.

So, K is a constant, so $1/KI$ will take out. So, $1/K$ into d/dx of the numerator which is dE_c/dx , at that time I can keep the Tl outside $+E_c + E^2/2Mn - E_f$ into d/dx of $1/Tl$, k

comes out as a constant. So, now if I put this term here I will find that the K is going out of the picture, the K is getting cancelled. Further, what is dE_c/dx . Now, you know that the force is negative gradient of potential energy.

Yes, okay, thank you for pointing that out. Here I have written dE_c/dx and I forgotten to put dE_f/dx , so let me put that in there. So dE_c/dx is nothing but - of f. So, you see here we are getting - of f/K times T_L and here you have f/K times T_L . So that is how this will get cancelled. So, let us assume that this has been put here and then let us cancel out the terms which go out.

So, f/K times T_L that is what you have here, this will cancel out with this term, okay, so f goes off. In other words, this term goes off. I am not removing K times T_L because it is multiplying this term dE_f/dx . Okay, then let me put this terms here the K when I am can cancelling this K, I can cancel this K also and again cancel this K here.

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$$-\frac{1}{T_L} \frac{dE_f}{dx} + \left(E_c + \frac{p^2}{2m_h} - E_f \right) \frac{d}{dx} \left(\frac{1}{T_L} \right) = 0$$

should hold for all values of p $\rightarrow -\frac{1}{T_L^2} \frac{dT_L}{dx}$

\Rightarrow each of two terms = 0

$\frac{dE_f}{dx} = 0 \quad \frac{dT_L}{dx} = 0$

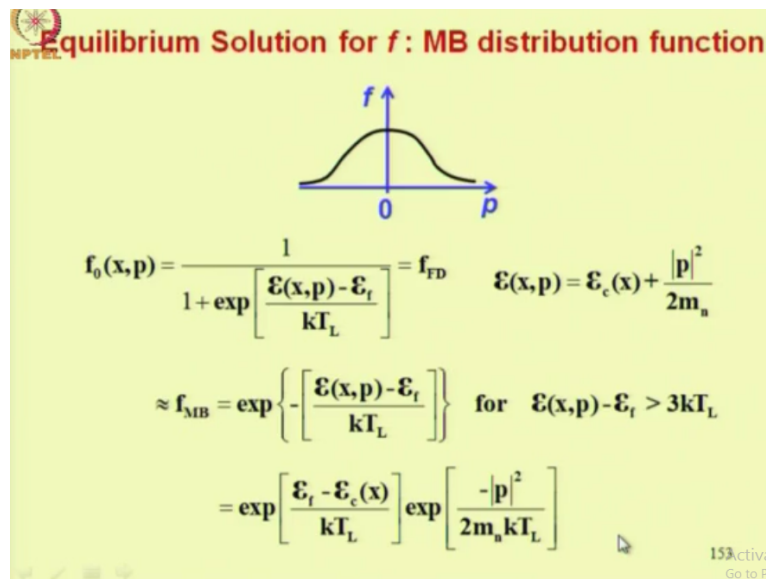
So, my equation will therefore become this dy/dx is nothing but $1/T_L$ into dE_f/dx with a negative sign + this quantity multiplied by dy/dx of $1/T_L$ and this is = 0, okay? Now, since this relation should hold for all values of P, all values of momentum. The only way you can have this = 0 is each of the term should be 0. Now, since T_L is non 0 the only way this will work is that $dE_f/dx = 0$ and dy/dx of $1/T_L = 0$, which is nothing but d of $T_L/dx = 0$.

So if you want d/dx $1/T_L = 0$, it is nothing but $-1/T_L^2$ square dT_L/dx . So, T_L is non 0, therefore, in fact $1/T_L$ is not 0. So, dT_L/dx should be 0. So, this is what you get is the condition. In other

words, this function is a solution of the Boltzmann's Transport Equation under equilibrium if $df/dx = 0$, $dT/dx = 0$. Now, that is a great result we already know that the Fermi level should be constant with x under equilibrium or constant with position and temperature should be uniform.

So, the Boltzmann's Transport Equation gives you this result, which we have obtained from some other method. It also tells you that this equation is a solution.

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The slide shows a graph of the distribution function f versus momentum p . The curve is a symmetric bell shape centered at $p=0$. Below the graph, the following equations are presented:

$$f_0(x, p) = \frac{1}{1 + \exp\left[\frac{\mathcal{E}(x, p) - \mathcal{E}_f}{kT_L}\right]} = f_{FD} \quad \mathcal{E}(x, p) = \mathcal{E}_c(x) + \frac{|p|^2}{2m_n}$$

$$\approx f_{MB} = \exp\left\{-\left[\frac{\mathcal{E}(x, p) - \mathcal{E}_f}{kT_L}\right]\right\} \quad \text{for } \mathcal{E}(x, p) - \mathcal{E}_f > 3kT_L$$

$$= \exp\left[\frac{\mathcal{E}_f - \mathcal{E}_c(x)}{kT_L}\right] \exp\left[\frac{-|p|^2}{2m_n kT_L}\right]$$

Now from the first level course you know that this particular function is nothing but the Fermi–Dirac function FD. So the Fermi–Dirac function is a solution of the Boltzmann's Transport Equation under equilibrium. However, now how do we get the shape like this? So, normally we use a Maxwell-Boltzmann approximation of this Fermi-Dirac function and if you plot this function it will give you the shape after substituting for E in terms of the potential energy and P square/ $2Mn$.

So, suffix MB stands for Maxwell-Boltzmann distribution. Now, when does this approximation hold from the first level course you know that if $E - E_f$ is more than 3 times kT_L , so $E - E_f$ here is more than 3 time kT_L . In other words, this quantity is more than exponential of 3 then within 5% error you can replace this whole function by simply exponential of minus of this quantity that is what we shown here.

And we write this as show here, so we separate out the exponential of $-P$ square/ $2Mn kT_L$ term which is contributed by this kinetic energy term and the other quantity. Now, when you

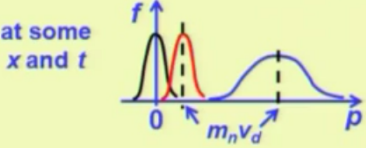
plot the distribution function f as a function of P , this is the term that has this particular shape, okay? You know that this is Gaussian kind of shape. Its peak is at $P = 0$.

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

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

at some x and t



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

Using 3-D version of the above approximation

$$n(r, t) = \frac{1}{\delta V} \sum_{i=1}^M f(r, p_i, t) = N_c \exp\left[\frac{\mathcal{E}_{fn}(r, t) - \mathcal{E}_c(r, t)}{kT_n(r, t)}\right]$$

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Now, we said that one approach to solving the Boltzmann's Transport Equation is to take the equilibrium distribution function and perturb it to accommodate the happenings of non-equilibrium case. So, what is happening in non-equilibrium? So we know that under equilibrium the entire carrier population has no net motion in any direction or no drift velocity,

or in general no directed velocity because your current could be because of drift diffusion, thermoelectric current, anything, right? So, let us say directed velocity. So, under equilibrium there is no directed velocity or there is no momentum P , right average momentum P is 0.

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So that is what in fact you can see the equilibrium distribution function is like this. This is P and this is 0 , so E_1 about 0 this is F_0 . The effect on non-equilibrium will be to introduce a directed velocity. You can do that very easily as follows. Let us first plot the situation under equilibrium. Now the disturbance is that there is a directed velocity. Now that is shifting the momentum or there is a non 0 momentum, average momentum.

Therefore, the distribution function is shifting to the right, to display the average momentum, non 0 momentum. This average momentum nothing but effective mass multiplied by the directed velocity. Under Quasi-equilibrium you find that the shape of the distribution function about the mean value is remaining the same, if the disturbance from equilibrium is small. We will shortly see what this means.

So, here is your distribution function corresponding to the red curve. The difference is that now P square has been replaced by $P - M_n v_d$ square. Now the quantity is which vary with x and t are all indicated in this equation. Quasi-equilibrium is characterized by the condition the electron temperature $T_n =$ the lattice temperature. We have already introduced the concept of carrier temperature.

And how the population of carriers can have a different temperature than lattice under non-equilibrium. Now if the carrier temperature is approximately called to T_1 then it is Quasi-equilibrium, you know that or other way around, in under Quasi-equilibrium T_n is approximately $= T_L$. In equilibrium $T_n = T_L$. So, this is the formula that is more general. Another change that has been done is the Fermi level is replaced by the Quasi Fermi level.

You know from the first level course, that, under non-equilibrium condition the Fermi level is replaced by the Quasi Fermi level concept. Now, what happens if the equilibrium, if the deviation from the equilibrium is large how do we accommodate that effect. So, in terms of the curve the large deviation from equilibrium is reflected in spreading of the curve, right. So, here the peak is sharp but under non-equilibrium the peak is broad.

So, more and more carriers are taking up momenta on either side of the average value. Now this effect is captured by changing the quantity T_n . So, in non-equilibrium T_n becomes more than T_L . How does T_n become so, how does this T_n becoming more than T_L broaden the peak, well that is seen easily. If this denominator is large, then this width of the peak region will increase, this clear from the nature of the Gaussian function.

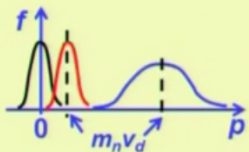
Now using a 3D version of the above equation, so here we have written terms as a function of x . 3D version this x is replaced by r . So one can derive so we are not doing the derivation, we are just showing the results using the same formula that we have introduced for carrier concentration and current density in terms of the distribution function. One derives this expression for carrier concentration, which we have derived in the first level course from a different starting point. So N_c and exponential of $F_n - E_c/kT_n$.

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

$$f(x, p, t) \approx \exp\left[\frac{E_{fn}(x, t) - E_c(x, t)}{kT_n(x, t)}\right] \exp\left[-\frac{|p - m_n v_d(x, t)|^2}{2m_n kT_n(x, t)}\right]$$

at some x and t



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

Using 3-D version of the above approximation

$$J_n(r, t) = (-q) \frac{1}{\delta V} \sum_{i=1}^M \left(\frac{p_i}{m_n} \right) f(r, p_i, t) = -qn(r, t)v_d(r, t)$$

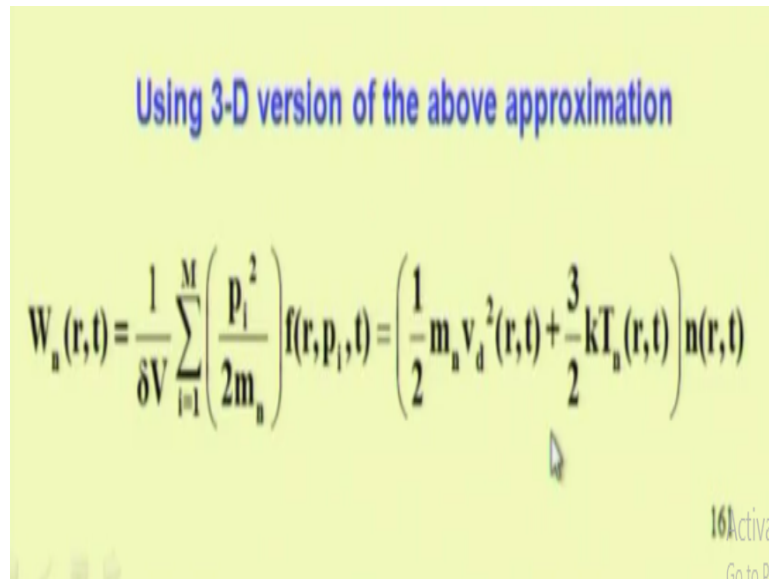
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The current density is given by this formula and operation according to this formula leads you to this equation. Q times, $-Q$ times carrier concentration N into directed velocity V_d .

Note that this is the average velocity as you can see from here. This average momentum and so the velocity correspondence to that is average velocity.

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Using 3-D version of the above approximation

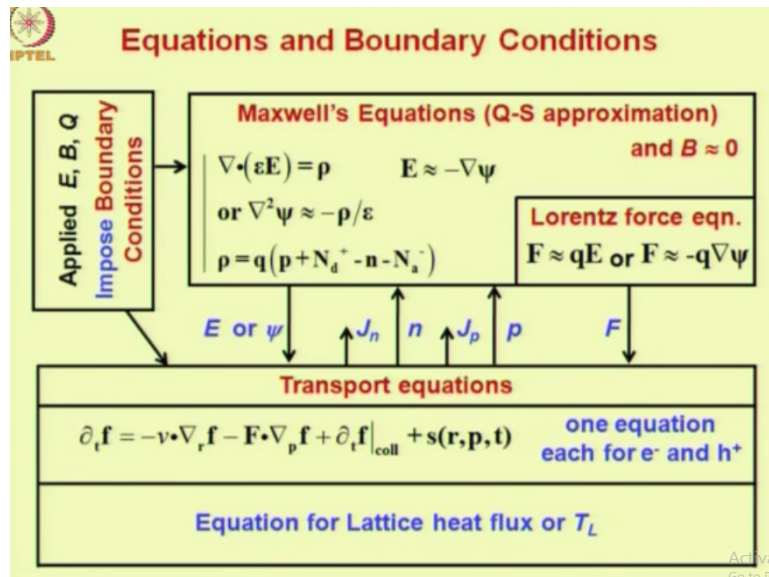
$$W_n(r,t) = \frac{1}{\delta V} \sum_{i=1}^M \left(\frac{p_i^2}{2m_n} \right) f(r, p_i, t) = \left(\frac{1}{2} m_n v_d^2(r,t) + \frac{3}{2} kT_n(r,t) \right) n(r,t)$$


Similarly, one can derive the kinetic energy density using the formula that we introduced the result of using this Displaced-Maxwellian Approximation is, that kinetic energy density = half Mn Vd square this the so called directed kinetic energy or drift energy and 3/2 times kTn which is the random kinetic energy or so called thermal energy and that is why you see the carrier temperature coming in here.

Now this multiplied by n, this multiplication n carrier concentration is coming, because this is not kinetic energy but kinetic energy density. Now, you would have appreciated by now why it is called a Displaced-Maxwellian Approximation. Because this function the red curve or this broaden blue curve is nothing but a displaced version of the curve under equilibrium. That is why it is called Displaced-Maxwellian Approximation.

The displacement is shown here by introducing minus $-Mn Vd$ along with P. Let us now look at our equations and boundary conditions picture. We have now introduced the Boltzmann transport equation as an equation of carrier transport, okay? So when we put this equation in the organization of all the equations the picture is as follows;

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So, here you have the Maxwell's equations with Quasi-static approximation and magnetic field = 0. There are 2 equations $E = -\text{grad } \psi$ equation and then you have Lorentz force equation which gives you the force because of electric field or potential gradient. Now this force and the electric field that is given here is used in the Boltzmann transport equation to solve for the distribution function f .

So in fact this force is entering here and electric field is used to find out this force. Now you need one equation for electron and another equation for whole. So you have 2 Boltzmann transport equations, one for electron other for whole. We are following the equation for electrons to explain the various aspects. Now what is interesting is to see that you need another equation here and that is the equation for Lattice heat flux or T_L .

Now this is because in our Displaced-Maxwellian Approximation you find the carrier temperature T_n coming there in the distribution function, and therefore you need to know that carrier temperature if you want to solve various quantities of interest. Now how do you get the carrier temperature? The carrier temperature depends on the lattice temperature, right? So, I need an equation to solve for the lattice temperature.

and this is the so called equation for heat flux Q . Recall that in the beginning of the discussion on the carrier transport towards the early lectures we had said that the carrier transport can be regarded as the consequence of 6 couple fluxes namely the electric flux, the magnetic flux, the heat flux, then electron flux, the whole flux and the displacement current flux, okay?

So, heat flux Q that is something that we had not brought in so far. So now at this point you realize why you need an equation for heat flux. So because the Boltzmann transport equation of semi-classical carrier transport requires the knowledge of carrier temperature which depends on the lattice temperature and this lattice temperature is to be solved from the equation for heat flux.

So that is what is shown here. So this heat flux equation can be regarded as a part of the transport equations. You need to impose boundary conditions on these equations for solving. So the applied electric field or magnetic field or heat flux imposed boundary conditions. So heat flux may be applied or it may be generated within the device they have explained how heat flux can be generated.

You have a power device heat is dissipated near the junction, right? So temperature of the junction is high compared to the base of the junction, right? And therefore there is a temperature gradient and there is a heat flux. Let us write down the equation for heat flux. Now we will not derive the equation but using our approach of Enology wherein we try to relate all our transport equations to the whole continuity equation.

Because we know that these equations are nothing but all reflecting, conservation, balance or continuity of some physical quantity. So we will be going to adopt that approach and see what kind of an equation we can write for the heat flux.

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Transport equations	
$\partial_t f = -v \cdot \nabla_r f - F \cdot \nabla_p f + \partial_t f _{\text{coll}} + s(r, p, t)$	one equation each for e^- and h^+
$\rho c \partial_t T_L = \underbrace{\nabla \cdot [k(T) \nabla T_L]}_Q + E \cdot J + \mathcal{E}_i [R - G]$	

Now, let me show you the equation first and then familiarize you with the equation. So the equation for heat flux looks something like this. So left hand side you have the time derivative of lattice temperature multiplied by 2 quantities rho, which is the mass density of the material, semi conductor material and see which is the specific heat capacity.

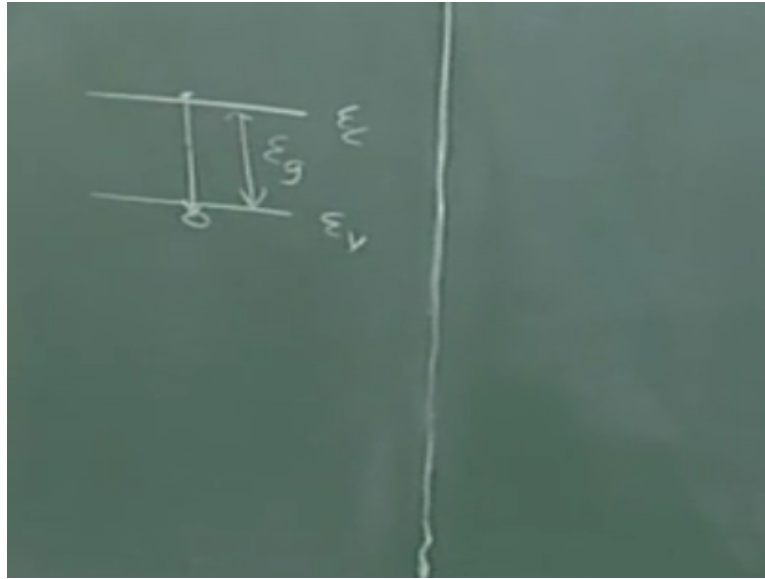
On the right hand side, you have divergence of the so called heat flux Q which is written as proportional to the temperature gradient T_l . The constant of proportionality is thermal conductivity which is a function of temperature and that is why this k has not been moved out of the divergence sign because it is a function of temperature and temperature can vary with x + source or sink terms.

Now one source of heat is the so called joule heating. So electric field multiplied by the current density. This is so called VI loss, right? You are applying a voltage and there is a current flow, V multiplied by I . So that has been disappeared as heat. So V into I is the total heat loss in the device whereas E into J is the heat generated within a local volume, right?

Now this is a differential equation which should work for different positions in the device, different local volumes and for different instance of time. So there is a microscopic description of the heat generation because of ohmic losses. Then you can have energy generated because of excess recombination. So $R - G$ is excess recombination. So if carriers recombine and if the mechanism of carrier recombination involves phonons then heat will be generated.

So we are writing here the recombination mechanisms which result in generation of phonons or heat in which the heat, means energy of recombination is dissipated as heat. Let us take an example of silicon, so the recombination mostly is dissipated as, energy dissipated as heat. So the rate of this excess recombination multiplied by the energy lost in each recombination that is the energy gap.

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So this is the diagram, E_c E_v and this the recombination, right, process in which the electron jumps into a hole and this energy gap. So, this energy that is released. Now let us show the correspondence of this equation with the whole continuity equation. Now here we are writing the term $G - R$ because the net generation or recombination for holes and electrons would be equal because the processes are always balanced, right?

Now the equation for heat flux, so here time derivative of T because the quantity analog is to $\rho_s T$, right hand side is spatial derivative of the flux because of temperature that is a heat flux Q and this Q we write as proportional to the temperature gradient. So in 1-dimension we are writing, so and you have a negative sign because the heat flows from higher temperature to lower temperature.

Just as the diffusion current of holes goes from higher concentration to lower concentration. So J_p/q if you write in the diffusion form it is dp/dx with a negative sign. Now this term for heat flux is analog as to this term of full current. So this is the Q here + the source terms, right? So that is E into $J+$ it is a recombination, net recombination which give rise to source of heat. So that is the term put here.

So this is analog as to this and these 2 terms together are analog as to this term. Now but dimensionally it is not yet correct. On the left hand side, you see you have a derivative with respect to time of the temperature. So dimensionally one can easily check that. I will have to put this mass density and specific heat capacity. So this is mass density which means mass

per unit volume that is kg per meter cube or gram per centimeter cube and this is specific heat capacity. This is thermal conductivity.

So this negative sign and this negative sign get cancelled, right? I leave it to you as an exercise to show that dimensionally now this equation is correct you put dimensions of these quantities and this is an exercise that I want you to do. Put dimensions of each of these quantities and show that this equation is dimensionally correct. There is another way to look at this Lattice heat equation.

The term ρc_T suffix L can be seen to be heat energy density. The left hand side is the time derivative of heat energy density and the first term on the right hand side is spatial derivative of heat energy flux. This equation can therefore be called Lattice energy balance equation in analogy to carrier energy balance equation which we shall consider in the next lecture. So, now what we find at this point is that we have a total of 3 equations.

3 equations of electromagnetic field and 3 equations of carrier transport. The equations of carrier transport consist of 2 Boltzmann's Transport Equations 1 for electron and 1 for hole and the equation for heat flux. So, the connection between the 2 sets of equations we shown here from the electromagnetic field equations you get the solution for the electric field or potential and from there you can get the force on an electron.

This information is fed into the transport equations which give us output the current density of electrons the carrier concentration of electrons the current density of holes and carrier concentration of holes. So, we have the 6 equations, okay at this point. However, the approach that we have just outlined allows you to only guess the form of the solution of the distribution function.

So, direct solution of Boltzmann Transport Equation is rather difficult, that is limitation of the set of equations that we have at this point. We can work to some extent with the displaced Maxwell form of the distribution function. However, certainly we would like to look for other alternatives of working with the Boltzmann transport equation. Because what we are interested in is not the distribution function itself ultimately.

But ultimately we are interested in the device current as a function of voltage. So, we want carrier concentration and current densities. That is our goal. So, can we get those quantities of interest without actually having to solve for the distribution function, as an intermediate step. Now that is what we want to explore, this takes us to the second approach.

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Solution of n , J_n from BTE

Approach 2

- The goal of modeling, n and J_n ,
 - are functions of four variables - x, y, z, t only
 - filter out detailed distribution of f over p_x, p_y, p_z
- BTE can be converted into “balance equations” for $n(x, t)$ and $J_n(x, t)$ by multiplying it with appropriate functions $\phi(p)/\delta V$ and then summing over all available states p ,

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

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The goal of modeling n and J_n are functions of 4 variables only x, y, z and t and filter out detail distributions of f over P_x, P_y and P_z . So, in the process of finding out n and J_n from f we are filtering out the effects of P_x, P_y and P_z . You know that from formula for the equations of n and J_n . Now that being the case, why not adopt this approach. The BTE can be converted into balance equations for carrier concentration n and current density J_n

both as a function of position and time by multiplying the BTE with appropriate functions, which are denoted as ϕ of P divided by the local volume δV . So, the functions we are considering are functions of momentum P and then summing over all available states P . This is your Boltzmann’s Transport Equation. So, we are saying that we will convert it into equation for n and J_n by multiplying each of the terms, with appropriate functions of P divided by local volume and then summing up. Let us see what we are talking about.

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$$\frac{\partial f}{\partial t} = -v \frac{\partial f}{\partial x} - F \frac{\partial f}{\partial p} + \left. \frac{\partial f}{\partial t} \right|_{coll} + S$$

$$n = \frac{1}{\Delta V} \sum_{i=1}^M f(x, p_i, t)$$

$$J_n = \frac{1}{\Delta V} \sum_{i=1}^M \left(\frac{-q p_i}{m_n} \right) f(x, p_i, t)$$

$$\frac{1}{\Delta V} \sum_{i=1}^M \frac{\partial f}{\partial t} = \frac{\partial}{\partial t} \left(\frac{1}{\Delta V} \sum_{i=1}^M f \right)$$

$$\frac{\partial}{\partial t} \left[\frac{1}{\Delta V} \sum_{i=1}^M \left(\frac{-q p_i}{m_n} \right) f \right] = \frac{\partial J_n}{\partial t}$$

So, this is our Boltzmann Transport Equation. You know that n is given by $1/\Delta V$ into $\sum f$ of x, p, i, t where you are summing up over all the available states or allowed states. J_n on the other hand is $1/\Delta V$ into now here you multiply by $-q p_i / m_n$, multiply the distribution function. Again you sum it up over. So, this is your expression for J_n and now this f here is the f here in this equation to avoid cluttering.

We have not put all the variables x, p, i and t for each of the terms here. Now how can I convert this equation into an equation for n , so clearly what I do is I simply sum f over the available states and divide by ΔV . While doing so what I have to do is I can put a sum here but then I know I will exploit the fact that I can interchange differentiation and summation.

So if I want n , I can go, do as follows, summing up $i = 1$ to M $\frac{df}{dt}$ is same as taking the derivative of the sum $i = 1$ to M of f . Now if I divide by local volume ΔV , I divide by local volume/ ΔV here also. Then this quantity, I can easily identify as $\frac{dn}{dt}$, okay. In fact, I can push the ΔV inside here further. I can write this as $\frac{dn}{dt}$, so I can identify it as $\frac{dn}{dt}$.

If I want J_n , I can take this do a similar thing. So what I do is I know that I can interchange summation and differentiation. So, I will use that facility and directly write the result. So, I can convert $\frac{df}{dt}$ as follows. So, I take the f , I multiply the f by $-q$ into p/m_n , then I divide by ΔV and I sum this. So, in the process what I am getting from this $\frac{df}{dt}$, is $\frac{dJ_n}{dt}$.


So, this is how, now this is the so called function of, this is the so called phi of P that we are talking about. In this case, the phi of P was simply = unity 1. Here phi of P is $-Q$ into P/Mn . So, this is how I can convert the left hand side into $\text{d}n/\text{d}t$ or $\text{d}Jn/\text{d}t$. Now what I will have to do is I will have to multiply all the terms by the appropriate function.

For example, if I want to write an equation for $\text{d}n/\text{d}t$ I multiplying everything by 1. So, this turns remain as it is and then I have to sum all of them all these terms over the states. In this case I have to multiply each of the terms here with this function phi of P and then do the summation. Division of by ΔV is not a big matter because ΔV will get even cancelled out in all the terms.

So, that is how I can get equations for n and Jn . I can convert this into equation for n and Jn . So, you see in this process I am not trying to solve the distribution function f . That is a great achievement of this approach, okay? And therefore I am not working with details of the distribution of carriers or momentum. You can see that when I sum up over the momenta the resulting function is a function of x and t alone.

So, this is a function of x and t . Though f is a function of x , p and t in the process of summing we have removed that. Similarly, Jn here function of x and t alone. So, we have filtered out P . We will develop this approach which is a powerful approach and which is commonly used today, in the next lecture.

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Summary of this lecture

Now, since we have come to the end of the lecture, let us make a summary of the important points. So, in this lecture we have discussed about working with the Boltzmann transport equation to determine carrier concentration and current density. So, one approach that we outlined involved trying to solve the Boltzmann transport equation analytically. Now this is very difficult,

so what we said is we could get a solution for f by guessing based on knowledge of the solution under equilibrium. Under equilibrium the Boltzmann Transport Equation becomes simple and it is possible to guess a solution for this simple equation. We guessed such a thing and we showed that the Fermi-Dirac function or its approximation namely Maxwell-Boltzmann distribution actually works very well under equilibrium.

It is a solution. Then we said that you can use this equilibrium function and modify it by making it a Displaced-Maxwellian function by introducing the directed velocity term in the equation which is the sign of non-equilibrium. In equilibrium there is no directed velocity no momentum. In non-equilibrium you have a net momentum or a directed velocity. So, we used, we introduced this term the resulting function was called Displaced-Maxwellian.

And we said by modifying the carrier temperature and using this directed velocity we can modify this distribution function at equilibrium sufficiently to manage the non-equilibrium conditions. Then we gave formula how you can use this function to derive n and J_n . We actually did not do the derivation but we showed how we can do that. However, in many situations Displaced-Maxwellian function is not a good approximation, right?

After all it is a guess work it is, an in spite guess work and approximate function. Therefore, we need to use alternate approaches and another approach we outlined was using the fact that n and J_n required for our device modeling actually does not need the detail distribution of momentum and therefore we can convert the Boltzmann Transport Equation into equations of n and J_n .

So, this approach we will develop in detail in the next lecture.