

Semiconductor Device Modeling
Prof. Shreepad Karmalkar
Department of Electrical Engineering
Indian Institute of Technology - Madras

Lecture - 09

Semi-classical Bulk Transport: EM field and Transport Equations

In the previous lecture, we began a discussion of the equations for modelling Semi-Classical Transport, so first we mentioned what is the organizations of these equations and boundary conditions, so we said that the equations of semi-classical transport can be divided into 2 sets one set is the electromagnetic field equations for electromagnetic field and the other set is the transport equation.

The equations of electromagnetic field they yield the values of electric field, the magnetic flux B and the force on an electron due to electric field and magnetic flux to yield these quantities the electromagnetic field equations require the knowledge of electron concentration, hole concentration, electron current density and hole density. Now these quantities namely n , p , J_n and J_p ordered by the solution of a transport equation which take as a input the electric field.

The magnetic flux and the force on an electron as inputs okay, so this is how the electromagnetic field equations and transport equations are coupled to each other we also mentioned that one should not forget about the boundary conditions. Because the non-contact and contact boundaries of the device impose conditions on the electric field, the magnetic flux and heat flux, so these are required for solving these equations.

Then, we discussed the equations of electromagnetic field in detail we said there are 5 equations which include 4 Maxwell's equations and one Lorentz force equation. Then we mentioned what are the approximations of these electromagnetic field equation namely the quasi-static approximation in which we neglect the time varying nature of electric and magnetic fields and we neglect in fact the magnetic field itself under these approximations electromagnetic field equations to - reduced to 3 equations namely the Gauss' law or the Poisson's equation.

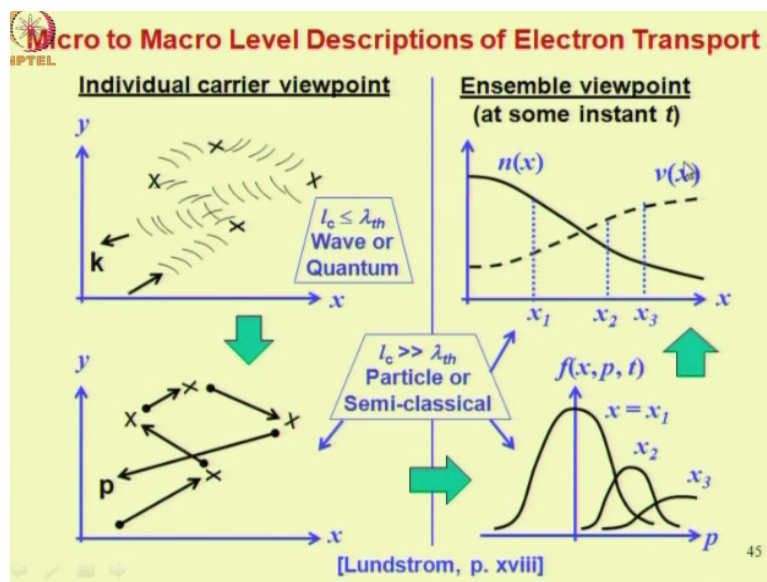
Then, the equation which relates electric field to the gradient of potential. And the Lorentz force equation which relates the force on an electron to the electric field, then we began the discussions of the transport equations we mentioned that because the situation in a semiconductor is very complex, there are a large number of carriers all colliding with each other and then there is a directed motions, superimposed or random motion.

There are variety of approaches to deal with this problem. Therefore, we have a large number of equations and different levels of equations. Now since we have a large number of equations we brought out an important point about these transport equations namely that most of them can be caused in the form of a conservation balance or continuity equation for example we took up the hole continuity equation which you have done in the first level course.

And we pointed out what is its form it consists of a time derivative of a quantity on the left hand side, the special derivative of the flux of the same quantity on the right hand side and some source and sink terms and we said we will show that the transport equations that we are going to discuss will mostly be obvious form and therefore it is not at all difficult to become comfortable with the large number of equations.

Now, with this background, we proceed further in this lecture on the transport equations.

(Refer Slide Time: 03:56)



To start with let us discuss the micro to macro level descriptions of electron transport, so the microscopic level and the macroscopic or the gross level, so progressively how do we go from microscopic level the small scale to the large scale, we shall show 4 different levels of descriptions the most fundamental level we look at the device current in terms of the state of individual carriers regarding them as waves.

So this approach in which we regard the carrier as a wave is valid when the device size or the mean free path between 2 collisions is less than the average de Broglie wavelength of an average thermal carrier, the other 3 levels of transport would be semi-classical and these will be based on the assumption that the device size or the mean free path between 2 collisions is much more than the thermal average wavelength of an electron.

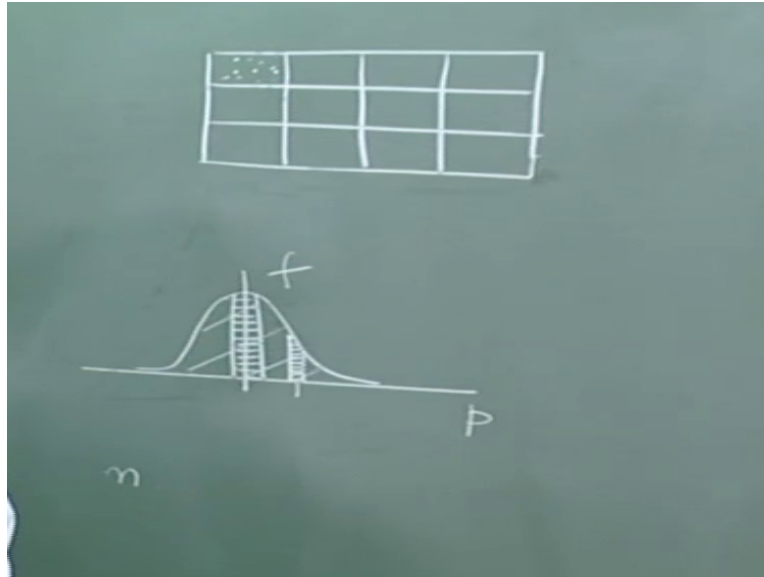
Let us look at the most fundamental level here we find out the current based on the status of individual carrier okay regarding the electron as a wave, so we take the group of electrons for each electron, we find out the state of electron by solving Schrodinger's equation and from the knowledge of this state we try to derive the current, as against this the next approximate level is that in which the carrier is regarded as the particle with an effective mass in between any 2 collisions.

So here we find out the state of the carrier using Newton's second law and based on the knowledge of this state which consists of actually a knowledge of the position of the carrier and the momentum of the carrier, so for each carrier we find out the position and momentum and from this description we try to derive the carrier concentration and current density.

The next approximate level is an ensemble viewpoint in which we regard the carriers or we treat the carriers in terms of their group so in this ensemble viewpoint the most fundamental level we look at the carriers from their distribution over the momentum, so this f here is the distribution function which is the function of position, momentum and the time instant okay, now let us explain this part in little bit detail what does the shape of a distribution function mean.

So in many cases the number of carriers in the device is so large that it becomes a complicated matter to analyze the state of each carrier and from there built-up the picture of the current, so instead of that we looking at the carrier as a group so now suppose this is our device.

(Refer Slide Time: 07:46)



and we divide this device in 2 local volumes like this now we look at a volume here and we look at the electrons which are present in this volume, now as we know all these electrons will not have the same momentum their amount will be distributed randomly, now what is the shape of this distribution that is what is given by this distribution function f , so what it says is that there is a certain momentum range in which there will be maximum number of particles.

And then beyond this value on the other either side the number of particles having larger momentum will be smaller and smaller and number of particles having smaller momentum then this value also will be reducing, so that is how you will get distribution like this for example in terms of the distribution function if I want to know the number of carriers then I can take this local value I will find that whatever electrons are there in this they will all be distributed like this.

So if I take the area under this curve and divide this area by the local volume then I will get the carrier concentration n just the area under this curve will tell me the number of carriers in this local volume, now in terms of this distribution function how do I know what is the current, so I

can find out the momenta's of different particles okay, for example I know that the number of carriers denoted by this area have momentum around this value.

A number of carriers denoted by this area have momentum around this value okay, so like this from a knowledge of the momenta's of different groups of carriers I can find out the current because after all we know that the current or current density is nothing but the momentum in a particular direction of interest, so this is the fundamental and ensemble viewpoint where we are treating the carriers in terms of groups.

And we are analyzing the momentum of distribution of this carriers and from a knowledge of this momentum of distribution we are building up the description of the carrier concentration and current density, the most gross level or microscopic level of description is in terms of carrier concentration and velocity v it turns out that the level of detail provided by the distribution function is not required in many situations.

All that we need in many situation is knowledge of how many carriers are present in local volume and what is the average momentum of this carriers we need not know the distribution of this carriers over momentum right, we need to find what is the average momentum of the whole group I can work with that for most applications now that is the approach that is the grossest approach and most commonly used.

So that is what is described here in terms of this diagram or illustrated here, so for example this distribution of electrons concentration n_x this line is obtained from the area under the curve here, so this diagram illustrates the distribution of carriers over momentum at 3 locations $x = x_1$, $x = x_2$ and $x = x_3$, so you find that the momentum average momentum is progressively increasing as you move from x_1 to x_2 to x_3 .

Because the peak point in this distribution function is moving to the right, so the average momentum information is in some other form the information about the average velocity of carriers therefore you find here that the carrier velocity is increasing as you increase with x , so at

x_1 the carrier velocity is this much that is a reflection of in fact that the peak is at some momentum here.

And this momentum whatever velocity you calculate from this momentum is actually what you put here at x_2 the distribution is like this so you take this value here on time value from there you find out velocity that you will get here and similarly for x_3 , so you find that the velocity increasing because here the reception function is moving to the right as you go from x_1 to x_2 to x_3 and on the other hand the area under distribution is going on decreasing.

And since the area divided by the local volume represented the carrier concentration therefore the carrier concentration is decreasing, so this picture about n_x and v_x is obtained by averaging of the picture that you have here and this picture in fact is sufficient to give you the current because you know that the current is given by the product of the electron concentration and the velocity and of course you multiply by the negative of the charge.



Now in some cases to analyze the transport phenomenon completely you may also need the knowledge of average energy apart from the average concentration, the average momentum in a local volume you may also need knowledge of average energy even that can be obtained from the distribution function and this we will see later, okay.

So to summarize we have given here 4 levels of description of carrier transport from microscopic level to microscopic level the most fundamental level is individual carrier view point with carrier as a wave, the next level is individual carrier view point but with carrier as a particle, then the next level is view point where you treat carriers in terms of an ensemble or groups and you look at the distribution over momentum.

And the most gross level you do not bother about the distribution over momentum but only bother about the average quantities such as carrier concentration, momentum and energy in a local volume and analyze the device in terms of these. Now we will proceed to outline each of these method of determining current in detail.

(Refer Slide Time: 15:10)

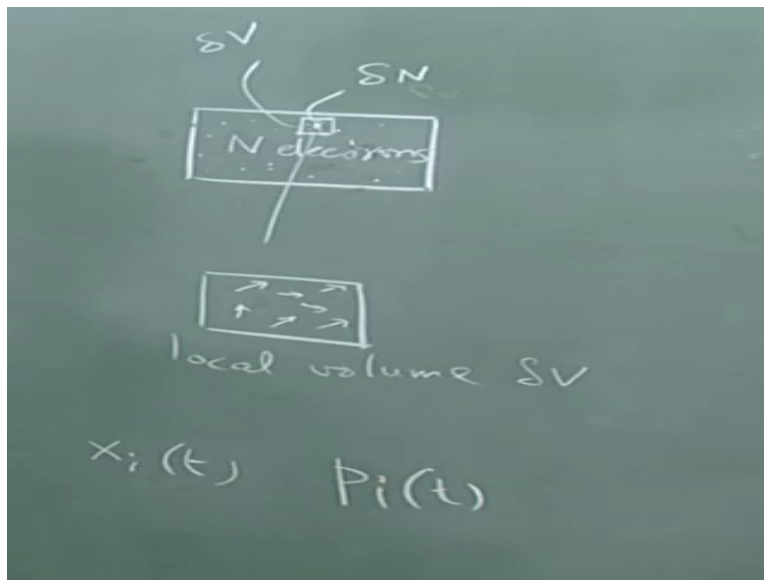
NPTEL **Transport Equations – Individual Electron Viewpoint**

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

53

Let us look at the transport equations from the individual electron viewpoint, so fundamental level is carriers as waves, the next level is carriers as particles, let us outline the steps in derivation of carrier concentration as a function of space and time and current density as a function of space and time. Let us assume that we have n electrons in the device so this is the complete device okay so in this whole device you have capital N electrons okay.

(Refer Slide Time: 15:47)



And we are looking at the steps of each of these electrons that is what we are doing here in this approach, if you regard the carriers as waves what you will do is the following, first you will solve the probability amplitude function $\psi_i(x, t)$ for each carrier i where i varies from 1 to n and

this is done using Schrodinger equation, now when you are doing this solution you will ignore the crystal potential and replace the mass of the electron in vacuum m_0/m_n .

So that the solution becomes easy, once you have obtained the probability amplitude function or the wave function for each carrier then you will use this formula modulus of ψ_i square for each carrier and sum it up for all the electrons and result will be the carrier concentration n , the carrier density J_n on the other hand will be obtained by summing up this quantity shown here by this equation.

Now let me clarify that at this point we are not discussing how these equations are derived right, we are simply outlining what is the procedure we will discuss meanings of this equation in detail a little later, so looking at this equation for J_n here let us explain the term this is \hbar cross divided by 2 times the effective mass and you have a j coming in here because the amplitude wave function is complex, now $\bar{\psi}_i$ is the complex conjugate of ψ_i .

So you are using a gradient here to find out the current, so very simply stated the current is nothing but current of electrons is nothing but the probability current because probability is varying between distance there is a gradient of probability, therefore you are getting a current you know that from your knowledge of Schrodinger equation the modulus of ψ_i square is nothing but the probability distribution function, more details about this equation we will discuss later.

Let us look at the next viewpoint individual carrier viewpoint wherein you regard the carriers as particles, now in this the first step would be to solve the state of the particle or electrons each of the electrons using the Newton's second law, so solve for the position $x_i(t)$ and momentum $p_i(t)$ and which is equal to effective mass m_n into the velocity and do it from Newton's second law. So while the state of a particle is described in terms of the amplitude wave function ψ_i which is the function of x and t .

In the case of the wave approach, in the case of the particle approach, each electron state is described in terms of its position x and momentum p , so this is what you are solving from

Newton's law. Now what you do is after you solve for the position of all the N electrons and the momenta of all the electron by Newton's second law at any instant of time identify the delta and electrons having their location x_i 's in local volume Δv .

So these are your N electrons and now this is your let us say local volume in that you find out what is the number okay, this local volume is chosen around the point at which you want to find out the carrier concentration and the current. So Δn electrons are the electrons in this local volume and you are obtaining this number by counting how many electrons fall into this local volume okay, now similarly let us say the local volume is ΔV .

So if I divide these ΔN electrons/ ΔV I will get the carrier concentration at this point, so that is what we are saying here carrier concentration $n = \Delta N/\Delta V$, now you can get the current density also from this information. Now for this ΔN electrons find out what are their momentum p_i and then sum up their momenta after dividing by the effective mass so that you get the velocity is essentially here.

And then you will divide by the local volume which incorporate those ΔN electrons and you get this current J_n , so here we are saying that find out the momenta's of each of this ΔN electrons okay, so if I expand this picture so it may be something like this. So this is the local volume in which you have these electrons in each electron has some momentum, so you are solving for this momentum from Newton's law.

Then, you are summing up all these momenta okay that is what you are doing to get the current density of course you are dividing by the local volumes so that your current density comes out in the proper dimensions.

(Refer Slide Time: 21:48)



Newton's 2nd Law

$$d_t p(t) = F(x, t) \quad \text{or} \quad m_0 \left(\frac{d^2 x(t)}{dt^2} \right) = F(x, t)$$

↓
This form reflects conservation of linear momentum

Now, let us look at the particle approach in some detail the most fundamental approach is actually the wave approach however the wave approach is sophisticated and it helps to discuss the particle approach first to understand the wave approach much more easily much more comfortably, so that is why the most fundamental approach is wave approach we are discussing the particle approach the individual carrier viewpoint with carrier as a particle first.

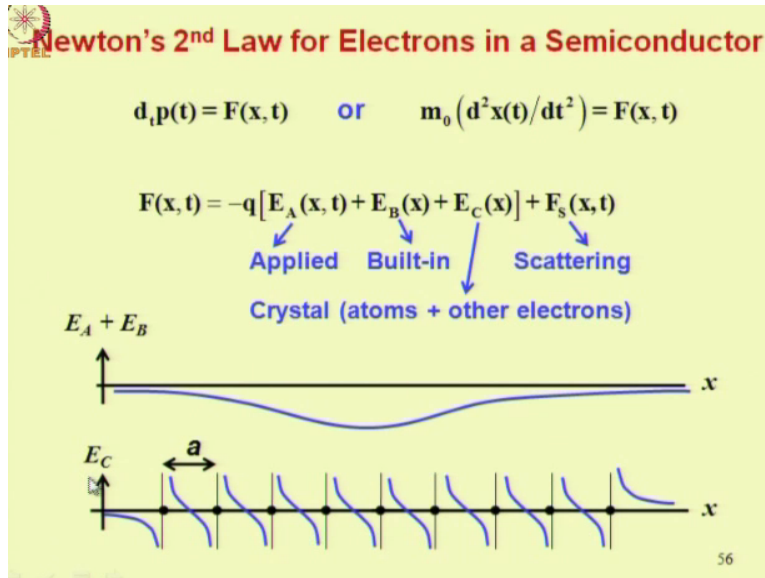
Now in this approach the state of the particle is solved using Newton's second law, so let us look at the Newton's second law it says rate of change of momentum with respect to time is equal to the impressed force when you write the Newton's second law in this form it reflects conservation of linear momentum, so we have said that our transport equation will all be some form of conservation or balance equations or continuity equations.

Then we also said they will have the form of the familiar hole continuity equation wherein you have a time derivative on the left hand side and the space derivative on the right hand side, now where is the space derivative here you see you may write the force as negative gradient of potential energy okay, when you do that you have a space derivative on the right hand side.

Now in practice often, we use this form of the Newton's second law where in the rate of change of momentum is written as m_0 into $d^2 x/dt^2$ where x is the position of the particle is nothing but force is equal to mass into acceleration, here there is a transit assumption that the

mass is not changing with time it is constant that is why it has been removed outside the differentiation operation, and this is equal to force.

(Refer Slide Time: 23:46)

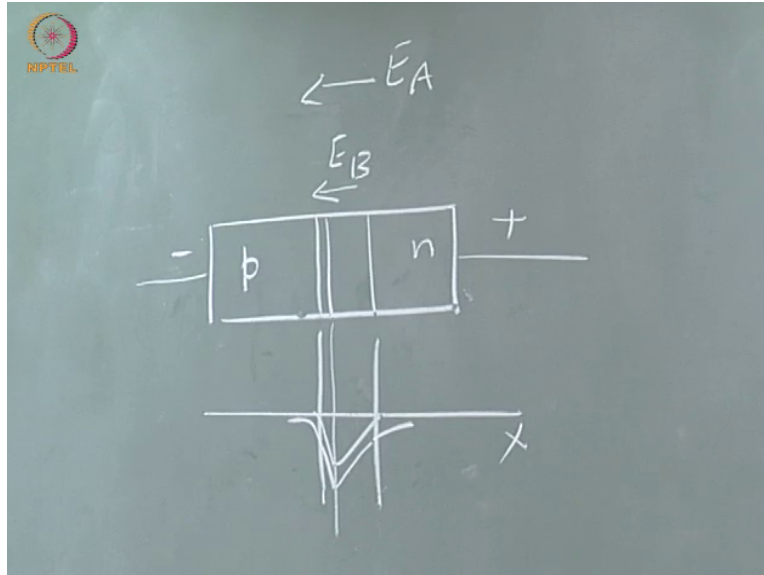


Let us look at the Newton's second law for electrons in a semiconductor in other words we want to see what are the forces acting on an electron in a semiconductor, now this is what is described here in this equation the force on electron can be due to applied electric fields or built-in electric fields or the crystal forces which includes the atoms, the nuclei positively charged nuclei and other electrons or holes okay it can be other carriers here more generally.

Then the force there is additional force apart from these forces namely the scattering forces, so while the forces due to applied electric field, applied built-in field sorry built-in field and crystal forces electric fields are expressed in terms of the electric fields, the scattering force has been simply left in terms of the force itself this the random force okay, now let us see some example of how this applied, built-in and crystal potentials or crystal fields how they look like.

Now here is the typical variation with x of $E_A + E_B$ and below that you have the crystal potential as a function of x , first let us look at this $E_A + E_B$ how do you get a shape like this.

(Refer Slide Time: 25:34)

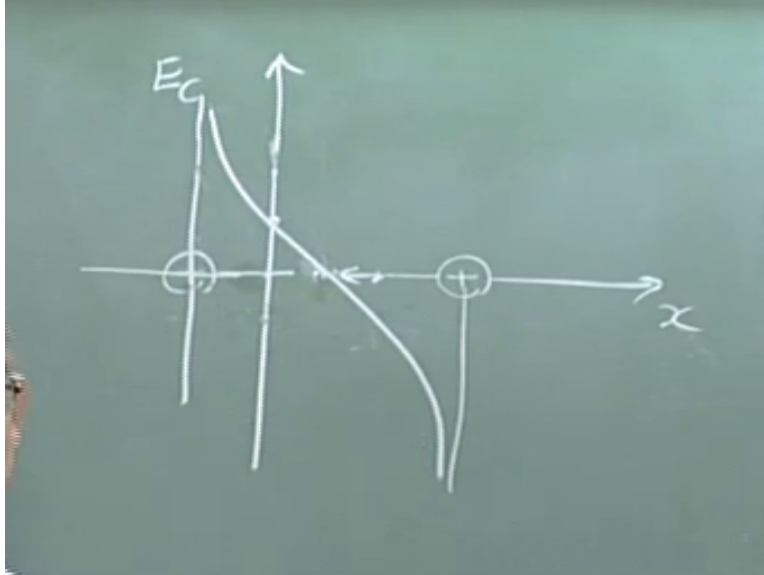


Supposing you take PN junction and this is the depletion layer supposing you are looking at the picture under equilibrium, then you know that there is a field from right to left n to p region this is built-in field and if I plot that field it will look something like this as the function of x over and above this I am superimpose and applied field for example if I am applying a reverse bias then I am superimposing an electric field in this direction because of the applied bias.

So effect of this also will get added here and so this electric field picture will move down okay will be this area will increase something like this and then you will have fields going here okay, so that is how you are getting a shape like this for the applied electric applied and built-in electric fields here, now let us look at the shape of the electric field due to the crystal atoms and other electrons or holes, how do you get a shape like this.

First, let us look at the field between any 2 nuclei because of the nuclei alone, so you have a positive charged nucleus at this point and another positively charged nucleus at this point okay, let us see what is the field picture.

(Refer Slide Time: 27:12)



Supposing, I have a positive charge here and I have another positive charge here, now I want to plot the electric field between these 2 charges supposing I take a test charge and it is somewhere here it will experience a repelling force from this point which is in this direction and it will have experience a repelling force because of this charge but the repelling force because of this charge will be smaller than this because this charge is closer to this charge.

So therefore the other force can be shown with the shorter arrow so the net force therefore is in this direction positive direction, so therefore at this point if I plot the electric field it will be some positive value okay this is x and I am plotting with E_C crystal electric, if I move closer to this point then the field will be more, so that is how you are getting some sort of a shape like this if I move this side then my net force will change direction it will be in this way.

Because the force because of this charge will dominate over the force of this charge, so therefore your field will be negative at this point in this direction and that is why you will get shape like this okay so this is the shape, now you can repeat this for every pair of atoms and you can then adjust this picture by taking into account the effects of other electrons and holes, so you see there are millions of electrons and holes and you are looking at the force on a single electron.

This is so called single electron approximation that is how you analyze the carrier transport in a device, so effect of all the other carriers can be observed by adjusting this picture a little bit okay,

so the net effect is what we shown here so that is how this picture a field picture is arrived at the distance between 2 atoms is equal to a and here this is the one end of the crystal and here you have the other end.

(Refer Slide Time: 29:34)

Newton's 2nd Law for Electrons in a Semiconductor

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

$$F(x, t) = -q [E_A(x, t) + E_B(x) + E_C(x)] + F_S(x, t)$$

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

Now this picture is fairly complicated let us say we are working with this equation what approximation or simplification can be make, now you know that we make the significant approximation namely the effective mass approximation, to simplify the effect of fields on the electron, so in this approximation we ignore the crystal potential rapidly varying crystal potential.

So it turns out that the applied and built-in potentials very much more slowly than the crystal potentials okay, so the effects of the crystal potential therefore we are ignoring while solving but absorbing their effect in the effective mass, so when we cross out this $E_C x$ term we change the m_0 to m_n to accommodate the effect of this, this becomes the significant simplification because now we are dealt with we are left with only the slowly varying potential okay its effect can be analyzed easily, and of course this scattering potential.

(Refer Slide Time: 30:51)



Newton's 2nd Law for Electrons in a Semiconductor

$$\text{Solution of } m_n \left(\frac{d^2 x(t)}{dt^2} \right) = F(x, t)$$

Situation (1) An electron between two collisions in a uniform semiconductor under equilibrium, i.e. a free electron with an effective mass, m_n

• $F = 0$

• Initial conditions:

$$p(0) = m_n v_{th}$$
$$\sqrt{3 k T_L / m_n}$$

$$x(0) = 0 \text{ (arbitrary)}$$

• Solution:

$$p(t) = \underbrace{p(0)}_{m_n v_{th}}$$

$$x(t) = x(0) + \underbrace{\left[\frac{p(0)}{m_n} \right] t}_{v_{th}}$$

64

So now our equation has changed m_0 has been replaced by m_n , let us discuss how we solve an equation like this, so the first integration of this equation gives you the velocity at any instant of time and the momentum which is nothing but the effective mass into the velocity and the second integration yields you the position x of t , the initial conditions required for solution are the initial velocity or momentum and the initial position.

So p_0 and x_0 let us apply this procedure to a couple of situations the first situation we have is an electron between 2 collisions in a uniform semiconductor under equilibrium that is the free electron with an effective mass m_n , so we are considering a situation where an electron is not acted upon by any forces okay, crystal forces we are ignoring we are taking their effect into account in effective mass, okay.

We are only concerned with applied or built-in forces for that since we are talking in terms of the picture between 2 collisions the scattering forces are also not considered here now what will the solution look like for this case, so $F = 0$ so here right hand side you set = 0 then initial conditions are $p_0 =$ effective mass into the thermal velocity we are considering a semiconductor under equilibrium.

So this thermal velocity is given by square root 3 times the Boltzmann constant into lattice temperature divided by effective mass of course this quantity is under the square root sign now

let us assume that the initial position of the particle is 0 this is an arbitrary references that we are assuming, now let me just clarify one thing why is it important that the semiconductor be uniform now we said there should be no applied forces rather there should be no force on the electron.

Now we have said that the force on electron can be due to built-in fields or applied fields, so the non-uniform semiconductor will have a built-in field because of non-uniform doping so we are eliminating any such built-in fields by suggesting that the semiconductor be considered to be uniform in doping, now what is the solution, the solution looks like this so the momentum as a function of time is obtained as p_0 itself.

So the first integration of this equation with force = 0 gives you the fact that momentum remains constant and equal to the initial value, now the second integration gives you the position x of t and this varies linearly with time it increases so x of $0 + p_0 t / m_n$ which is nothing but the thermal velocity in to time that is how the position of the electron will change.

(Refer Slide Time: 34:31)

Newton's 2nd Law for Electrons in a Semiconductor

Solution of $m_n (d^2x(t)/dt^2) = F(x, t)$

Situation (2) An electron between two collisions in a uniform semiconductor subjected to a spatially uniform steady state electric field, E

- $F = \text{constant} = -qE$
- Initial conditions:
 - $p(0) = m_n v_{th}$
 - $\sqrt{3 k T_c / m_n}$
 - $x(0) = 0$ (arbitrary)

Solution:

$$p(t) = p(0) + F t$$

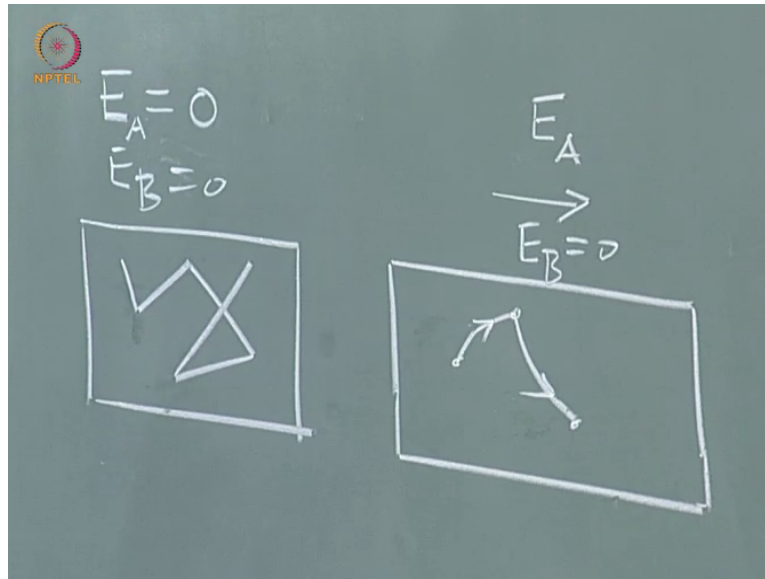
$$x(t) = x(0) + \underbrace{\left[\frac{p(0)}{m_n} \right]}_{v_{th}} t + \frac{1}{2} \underbrace{\left[\frac{F}{m_n} \right]}_{0.5(-qE/m_n)} t^2$$

Let us look at a more complicated situation namely an electron between 2 collisions in a uniform semiconductor but now subjected to a specially uniform steady state electric field E , so there is no built-in field in the semiconductor we are only having an applied field again we are not

considering the scattering forces because we are considering electron between 2 collisions. Now what would the picture look like now here F is constant = $-q$ times E .

First draw a diagram for this, so this is the picture, so this is the electric field that is applied E and there is exerting a force on the electron, now under equilibrium the earlier picture so the electron was moving like this okay.

(Refer Slide Time: 35:32)



So here you can see the position of the electron is changing linearly that is with time okay, so as when I follow electron between 2 collisions say between this point and this point its position changes linearly here equilibrium and $E = 0$, so both E_A is 0 and E_B is 0 because semiconductor is uniform here E_A is non-zero but E_B is 0 because this is uniform semiconductor. So effect of A is what we are trying to analyze now your initial momentum will be mn into v thermal where please note this carefully.

The thermal velocity can be different from the thermal velocity under equilibrium it is given by square root 3 times Boltzmann constant, the carrier temperature/ mn it is not the lattice temperature under equilibrium the carrier temperature is same as lattice temperature. But when you are applying a field, field could be high though it is study state and therefore the random velocity of carriers can increase over the equilibrium value okay.

So, that is what has been taken into account here the carrier temperature can be higher than lattice temperature, now as in the previous case let us assume that the initial position x_0 is 0 the reference is 0. Now what is the solution when you integrate this equation the first time when you integrate this equation the first time you will get the momentum where is linearly with time okay, the force is contributing to the increase in momentum.

This position of the particle on the other hand, varies quadratically so this = $x_0 +$ thermal velocity into t this nothing but p_0/mn into $t + \frac{1}{2}$ of acceleration forced by effective mass into a t square. This a familiar equation that we have come across in our school days, now what is the trajectory it looks like now if you see these portion which we are shown as straight lines would now look curve so when the electron is moving it would look like this right.

So this curved nature is coming because of the square law dependence on the temperature, on the time I am sorry on the time. Now similar approaches can be used in determining the state of the particle including the effect of scattering forces okay, supposing we are determined the position and the momentum of particles at different instance of time, so we have N electrons in the device these are the N electrons

And for all these N electrons we have to determine their positions x_i for different times and the momentum p_i at different times we have this information suppose using the procedure that we have just discussed, now how will you determine the current and the carrier concentration.

(Refer Slide Time: 39:07)



Estimation of $n(x, t)$ and $J_n(x, t)$ from the Particle Viewpoint

- At any t , the location $x_i(t)$'s of N electrons within the device, determined from Newton's 2nd law, yields the number δN of electrons in the local volume δV located at x , leading to

$$n(x, t) = \frac{\delta N}{\delta V}$$

- From a knowledge of $p_i(t)$'s of the δN electrons in δV , we derive

$$J_n(x, t) = \frac{-q}{\delta V} \sum_{\delta N} \frac{p_i}{m_n}$$

So let us look at that estimation of the carrier concentration as a function of space and time and current density as the function of space and time from the particle viewpoint, so at any t the location $x_i(t)$'s of N electrons within the device determined from Newton's second law yields the number of δN of electrons in the local volume δV located at x leading to this information about the carrier concentration at that x and at that instant of time $\delta N/\delta V$.

So again this is the picture this is local volume from a knowledge of $x_i(t)$ and $p_i(t)$ for all the N electrons I have find out the electrons which are present in this local volume then I take the ratio of this number to this local volume I get small n and similarly I find out the momenta's of this δN electrons and then from this information I will get the current, so that is the next step. From knowledge of $p_i(t)$'s of the δN electrons in δV we derive J_n of $x, t = -q/\delta V$ into $\sum p_i/m_n$ where the summation is done over the δN electrons.

(Refer Slide Time: 40:32)



Form of Equations

Assignment-3.2

Explain how Newton's second law

$$\frac{dp_i(t)}{dt} = F(x, t)$$

and Gauss's law for electric and magnetic fields

$$\nabla \cdot \mathbf{D} = \rho \quad \nabla \cdot \mathbf{B} = 0$$

represent continuity or conservation equations.

Let us now move to an assignment for you explain how Newton's second law $dp_i(t)/dt = F(x, t)$ and Gauss law for electric and magnetic fields that is divergence of $\mathbf{D} = \rho$ and divergence of $\mathbf{B} = 0$ represent continuity or conservation equations, so please show how these equations can be cast in the form of the hole continuity equation for example that is the assignment. Next let us discuss the individual carrier viewpoint in which the carrier is treated as a wave and see how we can determine the carrier concentration and current density.

(Refer Slide Time: 41:19)



Schrodinger Equation

$$j\hbar \partial_t \psi(x, t) = -\left(\hbar^2/2m_0\right) \nabla^2 \psi(x, t) + U(x, t) \psi(x, t)$$

- The action on the particle is specified by
 - potential energy (U) in Quantum mechanics
 - force ($F = -\nabla U$) in Classical mechanics

So here we use the Schrodinger equation, the Schrodinger equation is written out here on the slide let us just read it out once j which is the imaginary quantity square root of - 1 multiplied by \hbar cross multiplied by time derivative of the wave function ψ which is the function of space and

time = - of \hbar^2 cross square/2 m_0 into del square of psi + the potential energy function U which can vary with x and t in general and psi multiplied by psi of x, t so wave function psi.

Now the first step would be to familiarize ourselves with this situation and see it as of the same form as the hole continuity equation.

(Refer Slide Time: 42:30)

$$\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m_0} \nabla^2 \psi + U \psi$$

 Flux $\propto -\nabla \psi$

 $\psi \propto e^{j\omega t}$

 $\propto e^{jkx}$

So let me write the hole continuity equation $\frac{dp}{dt} = -\text{div } J_p/q$ that is the flux of p/dou x+ some generation and recombination rates okay, let us write down the equation for the Schrodinger and show that it coming out in the same form, so the quantity we are dealing with Schrodinger equation is psi which is the wave function, so we replace p/psi so we have a time derivative on this side.

Then the flux of p that is what is coming here so the flux of psi, now you recall in the previous lecture we had said the flux of a quantity can be put in 2 forms one is the product of the quantity into the velocity or other form is the flux is proportional to gradient of the quantity in turns out in the context of the wave function psi the flux due to the probability it depends on the probability gradient.

So the flux really depends the flux of probability is proportional to the gradient of psi, so the quantity here we should put in terms of the gradient of psi, now if you take the divergence of this

gradient of ψ then you will end up with a ∇^2 term right, now further flux is proportional to minus gradient of ψ because the current is from higher probability to lower probability just as the current is from higher hole concentration to lower hole concentration if you assume diffusion.

So when I take this negative gradient of ψ and take its divergence and put the negative sign this will get converted to ∇^2 so $+\nabla^2\psi$ is what is coming here, let us right now not bother ourselves with the constant that comes here we will put that later, now $+$ or $-$ whatever a source term now following this approach where you find that.

For example, the sink term here consists of the quantity p which is coming here for which we are writing the equation multiplied by a constant that is $1/\text{dop}$, so here similarly there will be a term proportional to the ψ and it turns out the proportionality here is the potential energy U , so this generates probability therefore there is a positive term this is a positive sign here, this quantity together represents some sort of generation or recombination source or sink.

So here we have a source the proportional to ψ therefore there is a source therefore it is a $+$ sign here, now let us complete the picture by putting the coefficients now U is potential energy, now you recall that the Schrodinger equation the right hand side terms can be regarded as kinetic energy and potential energy, so kinetic energy is written as in the classical terms square of the momentum by mass and momentum is of the form h cross k in the wave format.

So I can put here h^2 and when I take ∇^2 of ψ , since ψ depends on wave vector k multiplied by the x dimension I will get the k^2 term out of this so this is this quantity becomes $h^2 k^2$, so now divided by the mass so 2 times m_0 that is what is coming here, now when you come here on the left hand side to make a dimensionally appropriate we must put one h cross over there.

Now still it is not complete because you recognize that unlike p here the ψ is a complex quantity okay, therefore the when you differentiate the ψ will be having a function of the form $e^{j\omega t}$ for example we will discuss this point in detail later right now just accept from

facts, so where I take a time derivative of this quantity I will get a j out so one derivative I get one j out therefore you get a j here.

Similarly, the ψ also depends on the x in a similar form that is also a complex function e^{jkx} so when I differentiate this with respect to j sorry differentiate this with respect to x one differentiation will give me one j term and another differentiation will give me another j term, so product of j in to j , j square is -1 therefore you will get a negative sign here because there are 2 derivatives double derivative here with respect to x so that is what is the Schrodinger equation.

So you can easily see that it is of this form of the hole continuity equation right and therefore now here after we should not have any difficulty in remembering the various terms and how the various constants arise in that term in that equation, quickly some 2 points about this equation the action on the particle is specified by potential energy U in quantum mechanics but force F which is negative gradient of potential in classical mechanics.

So you see a Newton's law we used the forces to solve for the state of the particle whereas here in quantum mechanics in the Schrodinger equation you have the term U which is represents the action and this is nothing but the relation between this potential energy and force is what is given here, now that is a very interesting and important point that in quantum mechanics we always talk in terms of the potential energy that tells the action on a system whereas in classical mechanics you always talk in terms of the force.

(Refer Slide Time: 49:45)



Schrodinger Equation

$$j\hbar\partial_t\psi(x,t) = -\left(\hbar^2/2m_0\right)\nabla^2\psi(x,t) + U(x,t)\psi(x,t)$$

- This equation and Pauli's exclusion principle together explain most of the solid state phenomena
 - Planck's relation emerges from the time dependent part of the equation when U is a function of x only.
 - De-Broglie's relation emerges from the space dependent part of the equation when U is a constant, i.e. the particle is free from forces.



76

Just one more point this equation and Pauli's exclusion principle together explain most of the solid state phenomena, so like if you want to explain the phenomenon related to electromagnetic fields you have the 5 equations the 4 Maxwell's equation and the Lorentz force equation everything can be derived from there.

Similarly, if you want to explain phenomena based on quantum mechanics there are 2 things that you need to consider a Schrodinger equation and the Pauli's exclusion principle based on this everything can be explained now you might wonder so what happened to the de Broglie's relation and what happened to the Planck's relation, so de Broglie's relation is momentum = h/λ , λ is the wavelength of the wave.

And Planck's relation is energy $E = h$ times μ frequency of the wave, now we will show that the Planck's relation emerges from the time dependent part of the equation when U is a function of x only, so here if U is a function of x only does not depend on time then Planck's relation can be shown to emerge while solving the equation.

Similarly, de Broglie's relation emerges from the space dependent part of the equation that is this part here this is time dependent here you have time derivative and this is space dependent part of the equation when U is a constant, so you should set this U as constant that is the particle is free from forces, so de Broglie's relation applies only for a free particle okay.

Now this we will establish when we discuss the solution of the Schrodinger equation in the same way as we have discussed the solution of Newton's laws. Now we have come to the end of this lecture so let us quickly summarize the important points, in this lecture we continued our discussion of the transport equations, we explained the 4 levels of descriptions of carrier transport from microscopic level to microscopic level.

The most fundamental level was individual carrier viewpoint regarding the carrier as a wave, the next level was individual carrier viewpoint regarding the carrier as a particle, then the next level towards the microscopic level viewpoint was taking the carriers in groups and looking at them in terms of the distribution over momentum and the most gross level macroscopic viewpoint was looking at carriers within a local volume in terms of their average concentration, average momentum and average energy.

And we said that this macroscopic description in terms of carrier concentration, average momentum and average energy is the one that is generally applied in most cases, then the outline the procedure of deriving the device current and carrier concentration in the individual carrier viewpoint assuming the carrier to be a particle.

And we said we will do a similar exercise for the individual carrier viewpoint regarding the carrier as a wave and we just began this discussion and introduced the Schrodinger equation which is a fundamental equation in this particular approach we showed that the Schrodinger equation can be regarded as a conservation or balance equation which talks about the balance of probability and it can be shown therefore to be of the same form as the hole continuity equation

Now in the next lecture we will discuss the Schrodinger equation for electrons in semiconductor and also the solution of this equation and how to derive the current and carrier concentration.