Semiconductor Device Modeling

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Lecture - 10

Semi-classical Bulk Transport: EM field and Transport Equations

In the previous lecture, we have discussed the micro to macro level descriptions of carrier transport. So, we said the most fundamental level is individual carrier we appoint regarding the carrier as a wave. Then the next approximate level is individual carrier we appoint regarding the carrier as a particle. The next approximate view point happens to be the ensemble view point where we look at carriers as a group of particles or as ensembles.

We analysis the distribution of carriers within a local volume over the momentum. So, you take a local volume in a device look at the carriers in that volume and look at the distribution of these carriers over momentum. Then in terms of distribution function you try to find out the carrier concentration and current density. And the most approximate or gross level which is used very often is that you ignore the distribution of the carriers over momentum in any local volume.

Instead you only consider the average value of carrier concentration and average value of momentum in a local volume. And in terms of these quantities you try to modal the device. Sometime we need in addition to carrier concentration and carrier momentum or carrier velocity. The information about carrier energy as well so average carrier energy can also we used and it can be derived from the distribution function of electrons over momentum.

We outline in some detail the method that will be used to derive the current density and carrier concentration from the individual carrier view point regarding the carrier as a particle. So, we explain how you can use Newton Law’s and get the carrier concentration and the current. In this approach you are deriving the state of each individual particle using Newton’s law. The state is defined in terms of the carrier position and the carrier momentum.

So, once you get this information for every carrier we put this information together and get the carrier concentration and current. Then, we began a similar discussion for the development of explanations for carrier concentration and carrier density in terms of the state of the particle of the carrier obtained from Schrodinger equation. So, this is the individual carrier view point with carrier as a wave.

We mentioned a few points about the Schrodinger equation. Such as we showed how this equation can be regarded as a balance equation or a conservation equation of probability of carriers and we showed its correspondence to the continuity equation of the holes. Then we pointed out that while in Newton Law's we use force to specify the action on the electron in Schrodinger equation we use the potential energy function to specify the same action.

Finally, we pointed out that the Schrodinger equation together with Pauli exclusion principle are sufficient to explain most of the solid state phenomena based on quantum mechanical principles. The De Broglie wavelength, relation and the Planck relation we said could be derived from the Schrodinger equation, under certain conditions. Now, in this lecture let us proceed further and discuss the individual carrier view point based on the Schrodinger equation in some detail.

To begin with let us understand the Schrodinger equation for electron in a semiconductor. So, what are the forces or what is the potential that is acting on the electron in a semiconductor crystal.

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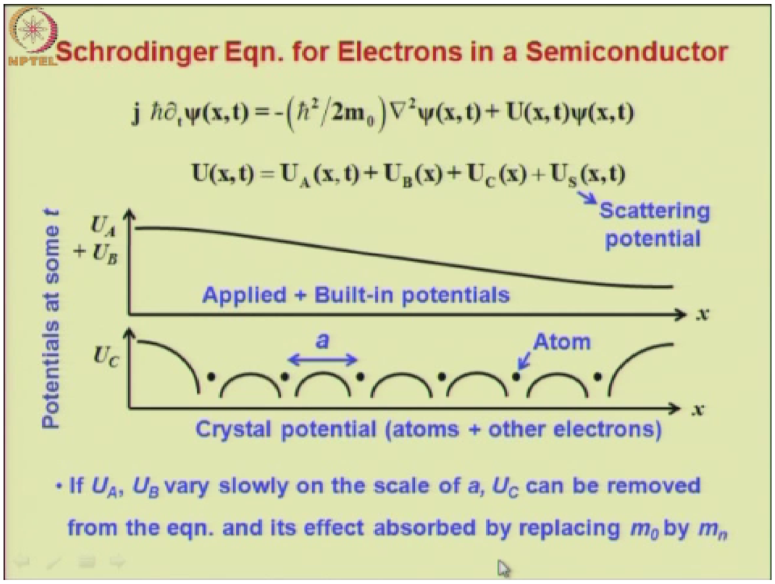

Schrodinger Eqn. for Electrons in a Semiconductor

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

$$U(x,t) = U_A(x,t) + U_B(x) + U_C(x) + U_S(x,t)$$

- If U_A, U_B vary slowly on the scale of a, U_C can be removed from the eqn. and its effect absorbed by replacing m_0 by m_n

So, the potential on an electron in a semiconductor crystal can be divided into these components. Each of these components corresponds to an electric field that we introduced in the context of analysis based on Newton Law's. So, UA is the potential because of applied electric field UB is the built in potential, UC is the crystal potential that is the potential because of positively charged nuclei and electrons and electrons and wholes other than the electron under consideration and US is the scattering potential.

Let us look at the shapes of these potentials. The applied and built in potentials together have a slow variation with x something like this. The crystal potential because of atoms and other electrons you can include other holes also here. However, shows a much more rapid variation on the length scale of the lattice constant. So, while the applied and built in potential is very slow. The crystal potential has rapid variations around the atoms.

We already explained how this kind of a shape results for a crystal potential when we were discussing the effective mass of electrons.

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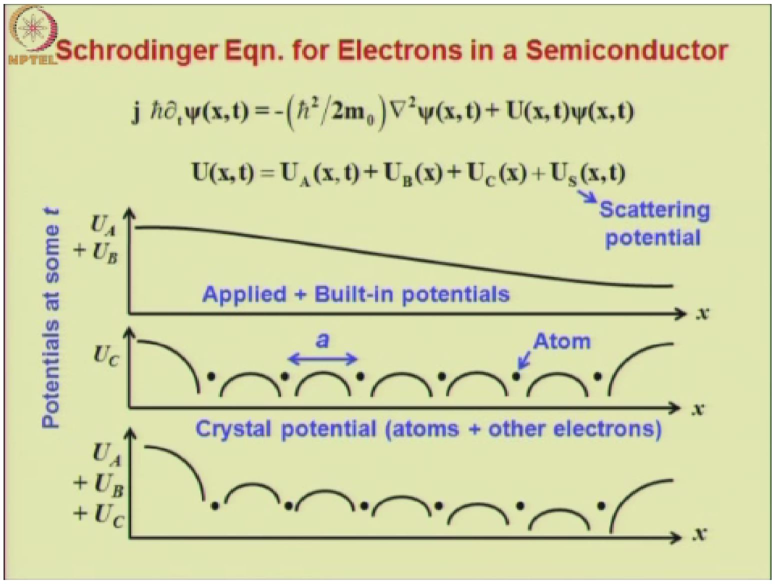

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$$U(x,t) = U_A(x,t) + U_B(x) + U_C(x) + U_S(x,t)$$

Now, when you put the applied built in potentials and crystal potentials together the picture looks something like this. Note, that all these potentials are being plotted at some instant of time. The scattering potential is the random potential that is not shown here that adds on to all these potentials. If UA and UB very slowly on the scale of a. This is the lattice constant here. UC can be removed from the equation and its effects absorbed by replacing m0/mn.

This is the concept of effective mass.

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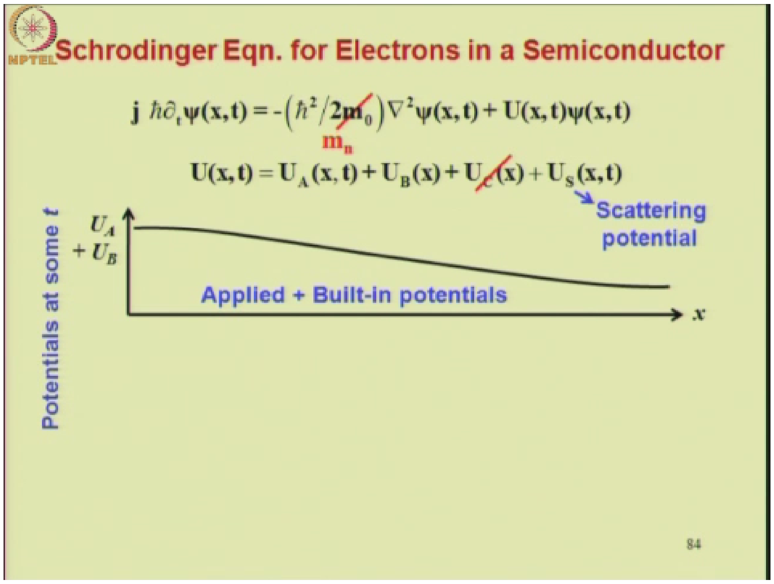

Schrodinger Eqn. for Electrons in a Semiconductor

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

$$U(x,t) = U_A(x,t) + U_B(x) + U_{\cancel{C}}(x) + U_S(x,t)$$

Scattering potential

So that is what is shown here on the slide we have removed the crystal potential and as a result the picture has become quite simple. So, you see you only have a slowly wearing built-in potential to deal with so UC has gone out of the picture and m0 has been replaced by mn. Now, let us understand how this kind of built-in and applied potential can result. We have explained with the example of the p-n junction when we discuss the development based on Newton’s law.

So, there we consider the electric field while here we can plot the potential for the same situation.

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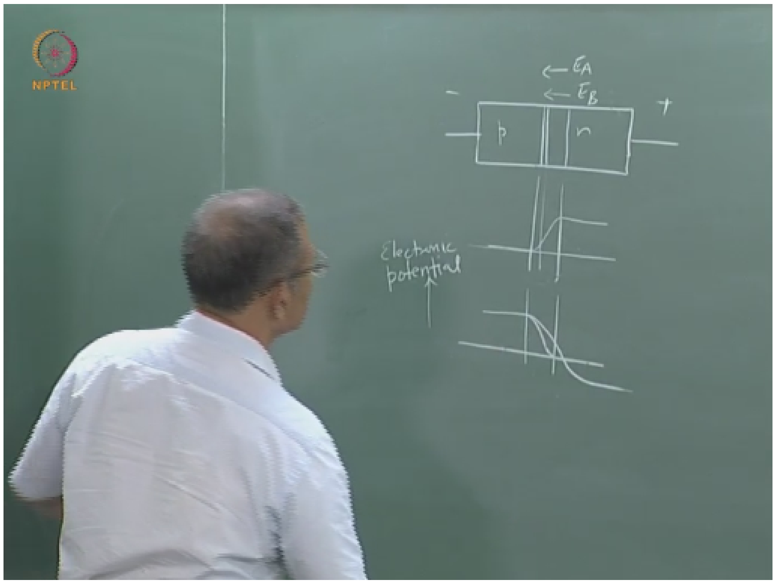

So, if you have a p-n junction and this is the space chart region so under equilibrium conditions if you sketch the potential, this is the built-in potential and it will appear to increase like this. Something like this. So, as you move in this direction the potential falls. Now, this is a potential due to a positive charge if you plot the electronic potential then it will follow exactly the mirror image of this a shape like this.

So, this is electronic potential. This is conventional potential. Now you can super impose a potential because of the applied voltage for example if you apply reverse bias then there is an electric field that super imposed on this and this special region expands and then the potential variation also increases. So, this potential variation here similar would increase. So, for example it could increase say something like this.

So anyway this tells you how you can get a shape like this for the electronic potential that is what is shown here. Now, let us look at solution of this Schrodinger equation.

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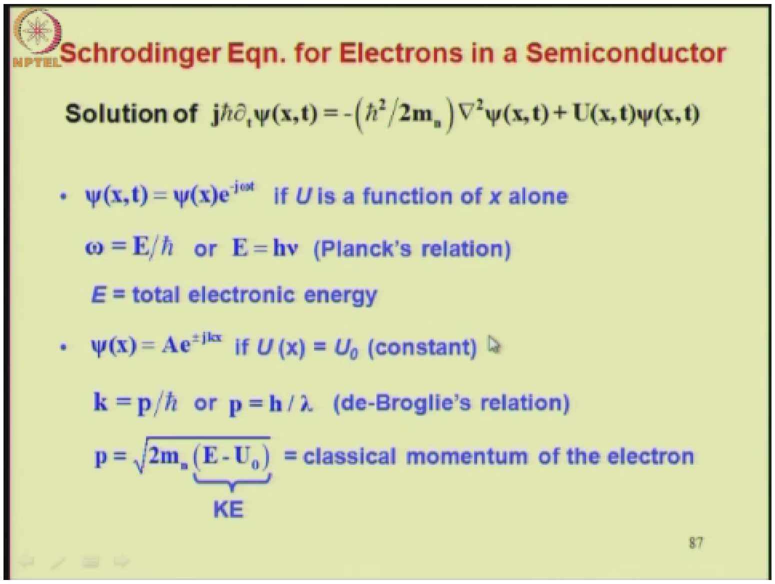

Schrodinger Eqn. for Electrons in a Semiconductor

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

- $\psi(x,t) = \psi(x)e^{-j\omega t}$ if *U* is a function of *x* alone

  $\omega = E/\hbar$ or $E = h\nu$ (Planck's relation)

  E = total electronic energy

- $\psi(x) = Ae^{\pm jkx}$ if *U* (x) = U_0 (constant)

  $k = p/\hbar$ or $p = h/\lambda$ (de-Broglie's relation)

  $p = \sqrt{2m_n\underbrace{(E-U_0)}_{KE}}$ = classical momentum of the electron

So, we are following the same approach that we have followed for the individual carrier view point based on the carrier as a particle and this analysis was based on Newton's Law. So, whatever we did for Newton's Law we are doing for Schrodinger equation. If U is the function of x alone so here U is a function of x alone so t goes out of the picture here than one can show that the wave function psi (x, t) can be shown as product of 2 functions.

One is a function of x and another a function of t and the function of t is of the simple form e power -j omega t where the omega the angular frequency of the wave is given by the energy of the electron divided by the h cross. Now, the same equation can also be written as E = h nu because omega is 2 pi into nu, where nu is the frequency. So, this is the so called Plank's relation.

Now, this is what we had said in towards the end of the previous lecture that Plank's relation can be derived from Schrodinger equation, is not an independent relation of quantum mechanics. Once you use Schrodinger equation as a fundamental equation. Now let us explain this point. Note that this relation is obtained only for the case when U is a function of x alone. So, let us show how if U is a function of x alone you get this kind of form of the solution of Schrodinger equation.

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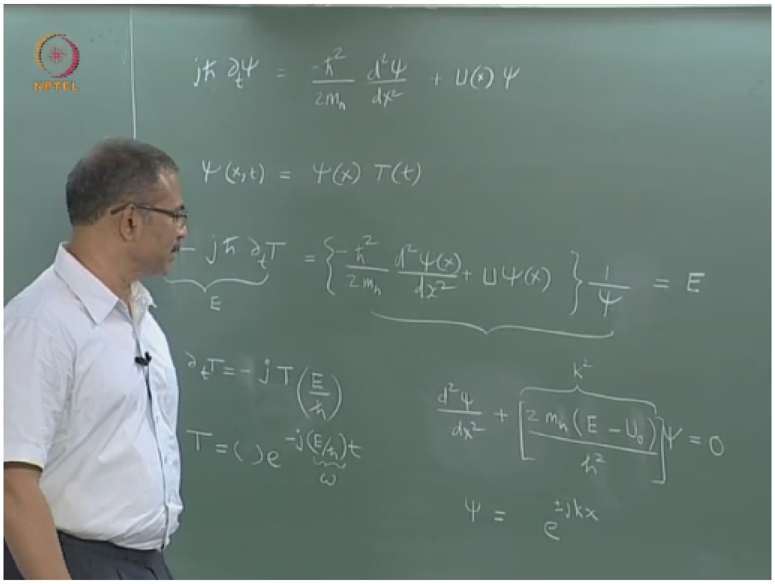

So, the Schrodinger equation is j h cross dou psi/dou t = -h cross square /2 into effective mass. Because we have removed the crystal potential out of the picture into let us write in one-dimension d square psi/d square+u which is a function of x alone into psi. Now, when this is the function of x alone we separate psi which is the function of x, t in the above equation into product of 2 separate functions.

One the function of x and other is the function of t. Now, how can you establish this well you assume this result and substitute in this equation and see what happens? So, if you assume this resultant substitute in this equation when I am taking a derivative with respect to time this psi x will not be coming into the picture and so left hand side will appear as j h cross dou T/dou T into psi x.

This is equal to on right hand side you will have -h square/2mn and when I am taking derivative with respect to x this thing will not come into the picture. So, you will have d square psi x/dx square and this we will keep it out for present. Plus, this psi is product of these 2 because this psi of x, t. So, here you will get psi x and that is T of t has been taken out. Now, I can rearrange this equation.

I can push psi x on this side and T of t small t to this side so 1/psi. Now, this side is a function of small t alone and this side is a function of x alone. So, both of these have to be equal to a constant and that constant turns out to be the energy of the electron. Now, take the time varying part of the equation that is this quantity is = E then you get T/E/h cross. So, I am shifting I am setting this = E.

So, T goes up and E also comes in the numerator and h cross comes in the denominator and then you have J coming in the denominator. So, I can put the j on the top and put a negative sign here. Now, the solution of this equation can be easily be shown to be of form T = e power -j into E/h cross into t of course into some constant coming there. So, you see this is where this thing is the angle frequency omega of the electron wave.

So, this is where you are getting the relation e / h cross = omega. Now, this is the explanation for this relation here. So, it explains how you get the Plank's relation from Schrodinger as equation for the condition U is the function of x alone. Now, what about the function psi of x? It turns out that if you assume U of x to be a constant independent of x then psi of x works out to be this form constant A into e power +- j times k times x.

Where k turns out to be equal to the momentum of the electron divided by h cross or when you transform this relation because k is 2 pi/lambda it come out as p = h/lambda that is the De Broglie's relation. And this p is a classical momentum which depends on the kinetic energy that is equal to total energy of the electron minus the potential energy. Now, let us establish this part how you get the De-Broglie's relation and how you get psi x to be of the form Ae+/-j k x.

For this purpose, we look at the same equation but now we work with side. So this part of the equation if you work with this part of the equation then it reduces us to this quantity is = E times psi. And transforming that your equation becomes -h cross square/2 mn into d square psi/dx square+, I am sorry here U was missing that I am introducing now. And that U you are going to write it as u0 because we are going to assume u is a constant with x.

Here U was a function of x but here we are going to make it a constant U0 -E into psi. So, this is = 0, right. But let us transform this as E- U0 because E is the total energy and U0 is the potential so that this remaining part will show the kinetic energy. So, we write it as E-U0 and there is negative sign here. There is a negative sign here also so both negative signs go away and again you have positive sign and this is 0.

So, this is your equation which you can further transform I can shift h cross square/2mn to this term. So, d square psi/dx square+2 mn into this quantity/h cross square into psi. Now I can all this quantity as, k square then the equation will be of the form d square/psi/dx square+k square psi = 0. Now, this is a very simple differential equation you know that its solution will consist of 2 component psi = e power jkx with either a positive sign or a negative sign.

Both solutions are possible, you know it will satisfy this equation. Now, let us put a constant A here, now what is this k? This K is the square root of this quantity. So, K = square root 2-time mn into e -U0 upon h cross.

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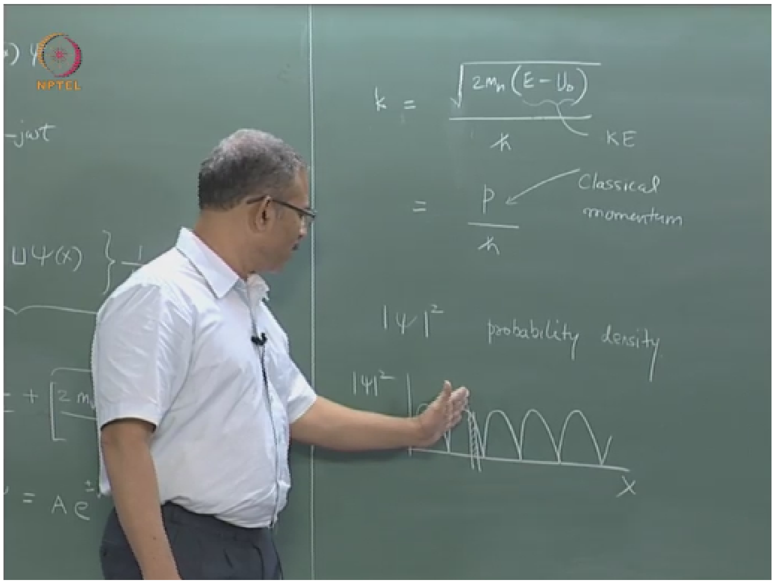

But this quantity here is nothing but the kinetic energy. The classical kinetic energy therefore the square root of 2mn into kinetic energy as you know, is equal to the classical momentum. So, therefore, you can also write this as the classical momentum p/h cross so classical momentum. And from here you get this relation that is shown on the slide. So, k = p/h cross or p = h/lambda. This is how we have shown how the de-Broglie’s relation arises.

And we have shown that for many situations we can use solution of the Schrodinger equation which has this form that is the psi of x, t separated into psi x into t of t where this is of the form e power - the omega t and for the particular case so this form works when your U is a function of x alone and phi of x can be shown to be of the form A constant into e power +/- j times kx. if this U is independent of x and is a constant.

So, these aspects will be useful for us when we discuss solutions of the Schrodinger equation.

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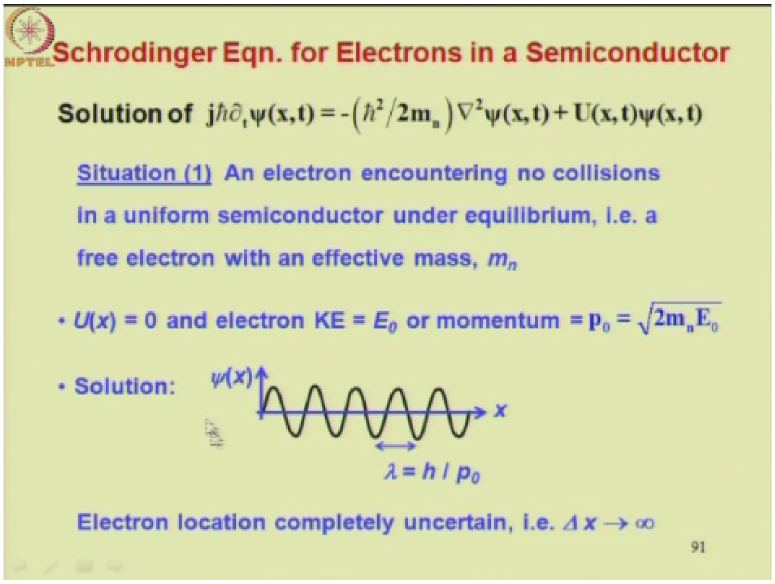

Schrodinger Eqn. for Electrons in a Semiconductor

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

Situation (1) An electron encountering no collisions in a uniform semiconductor under equilibrium, i.e. a free electron with an effective mass, m_n

- $U(x) = 0$ and electron KE = E_0 or momentum = $p_0 = \sqrt{2m_nE_0}$
- Solution:

Electron location completely uncertain, i.e. $\Delta x \rightarrow \infty$

Now let us take a particular situation an electron encountering no collusions in a uniform semiconductor under equilibrium that is a free electron with an effective mass mn. So, what is the solution? So, you will recall that we have discussed exactly the same situation when we applied the Newton’s Second law and try to derive the state of the particle. So, here we want to do it using the Schrodinger equation. See what is the difference?

So, U of x let us assume it to be 0 because there is no applied electric field there is equilibrium condition, so no applied electric field. No, built-in electric field as well because it is a uniform semiconductor and let us assume that electron has a kinetic energy E0 or a corresponding momentum p0 which is equal to square root of 2 times mn E0. The solution of this just now we discussed that form of solution so this has been plotted as a graph.

So, it is like a sign wave where the wavelength lambda = h/p0. Now, what do you derive from this information? We derive the fact that electron location is completely uncertain that is the delta x uncertainty in the location of the electron goes to infinity. Now, how do you derive it from this condition, from this solution Schrodinger equation for a free particle. So, here you have to invoke the physical interpretation of the wave function.

So, you will recall that the wave function psi by itself does not have a physical interpretation. However, its modal square that is the psi multiplied by its complex conjugate this has the physical meaning of probability density or probability distribution. So, if you take a one dimensional situation then if I plot the modal of psi square as a function of x. Let us say for the kind of problem that we are considering.

So psi as a function of x is a sign wave so psi square would look something like this and this will go on a x = infinity and on this side to xn into -infinity. Now, if I want to know what is the probability of finding an electron? Let us say within some interval like this at this location then there is under this curve that is the integral of psi square over the interval in which you find the electron.

So, this area indicates the probability that electron will occupy that location. Now, since goes from - infinity to + infinity it means that the electron can in principle be anywhere from -infinity to +infinity though it is true that there are more likelihood that it will be here or here or here near the peak locations where the probability density is maximum. But in principle it can exist anywhere.

So, now this is an interesting result that the Schrodinger equation has given us. According to this equation if you have a free electron which is not acted upon by any forces and you think that it has a specific energy or momentum then you cannot locate this electron anywhere its location is completely uncertain. So, this is what is hinting towards the problem. That if you regard the electron as a wave you cannot get its momentum and its location precisely.

If you try to give its momentum precisely then you do not know its location. Now, we are not comfortable with this kind of a thing because from our practical experience we would like to locate the electron at some point. Now let us see what happens if you try to locate the electron?

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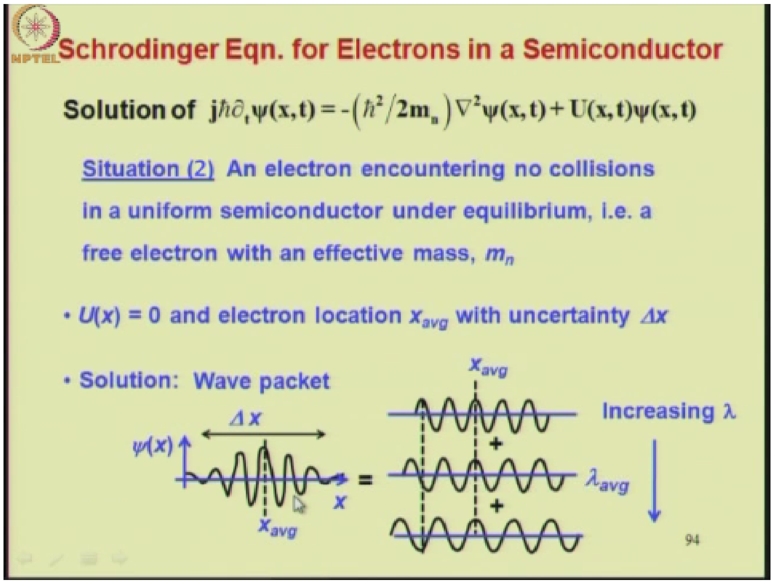

Schrodinger Eqn. for Electrons in a Semiconductor

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Situation (2) An electron encountering no collisions in a uniform semiconductor under equilibrium, i.e. a free electron with an effective mass, m_n

- $U(x) = 0$ and electron location x_{avg} with uncertainty Δx
- Solution: Wave packet

So, let us say that he potential energy is 0 it is a free electron and the electron location is X average with uncertainty delta x. So, we will not try to locate the electron precisely. First let us say we allow some uncertainty. Why? Because right now we are faced with a problem where the electron is not possible to locate at all anywhere? It can be anywhere? So let us go step-by-step let us say okay.

We will accept some uncertainty not so much of uncertainty from - infinity to + infinity but some uncertainty. Let us say we want to locate the electron at some x within the uncertainty delta x that location where we want to locate it is called average location, X average. Now, is he wave picture for this case? So in terms of the wave picture the psi x has the function of x would look something like this.

Because we interpret the wave function psi as a function whose amplitude square gives you the probability of locating the electron and since psi has to be alternating and therefore psi square is also is changing the only way you can locate an electron within some uncertainty, finite uncertainty is to have the wave function limited in some way to that region. Therefore, the shape of the wave function looks something like this.

So you can see that the wave function is dying out. It is maximum at x average and it is dying out. Now, this is the kind of solution you are looking for? Now, how can you get a solution of this sort starting from a wave which have a particular wave length. So, we know that

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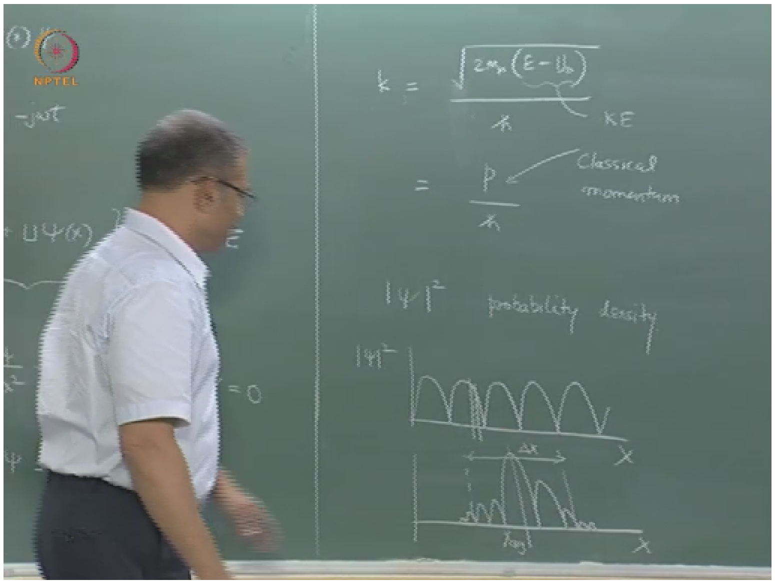

We have a wave like this. So if you psi of x is like this regular wave then we know that this wave corresponds to a particle which has the price momentum which is given by if this is lambda. The momentum p = h/lambda starting with this wave how do you get a wave which is maximum at some point and decays thereafter? In case, if the particle has to be located in some uncertainty would be something like it will be maximum here and then it will go on decreasing.

Same thing on the other side and this is the so called location x average and this roughly tells you the uncertainty delta x. So, to get this kind of wave packet, this is called wave packet because we will see that this can be compost from individual waves of continuous varying wave length so something like this. So you start with a wave which has an average wave length lambda average which corresponds to the energy of the particle, average energy of the particle.

So, if you have lambda average it will give you average momentum = h/lambda average.

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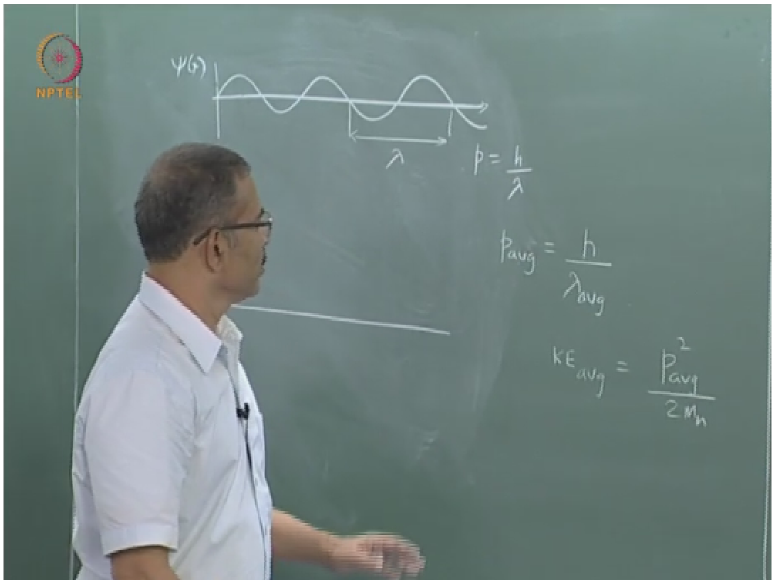

And therefore, you can associate a kinetic energy, average kinetic energy as P average square/ 2 times the mass. So, that is how you can choose the average wavelength for the given momentum or energy. And now you super impose on this wave, wave length less then lambda average and more then lambda average. So, you do super imposition as follows for all the waves let us locate their peaks at the location x average which is where we want to locate the particle.

And then, on either side, if you add the waves, you can easily see that as you move way from this point the amplitude of the sum of these waves will go on decreasing for example, look at the location here, you have a positive value then you have a negative value here and you have another negative value here a small negative value and more. So if you add these 2 the negative values will reduce the sum from the positive value.

And you go further and further away you will find that for a large number of waves the amplitude will randomly vary and therefore they will all sum up to very, very small value. So, that is how a packet of waves like this with continuously varying lambda around the average value. So, the lambda decreases from the average value as well as increases from the average value.

You add a large number of such waves the more and more waves you add the more rapidly this function will decay. So, supposing you want a function here which is very sharp you want to locate the electron very precisely and you want this kind of a function for psi square then you will have to add a very, very large number of waves. So, now what is the result you get? Since each wave like this has this corresponding momentum.

The various waves that you adding have their own momenta and therefore you are not getting a precise momentum you add up the momenta of all the waves so your momentum now is having uncertainty and as we have said the more precisely you want to locate the particle the larger the number of waves you have to add therefore, the larger is uncertainty in momenta. Because, all these are waves of different wavelengths therefore they are waves of different momentum.

Now, that is the important conclusion you get.

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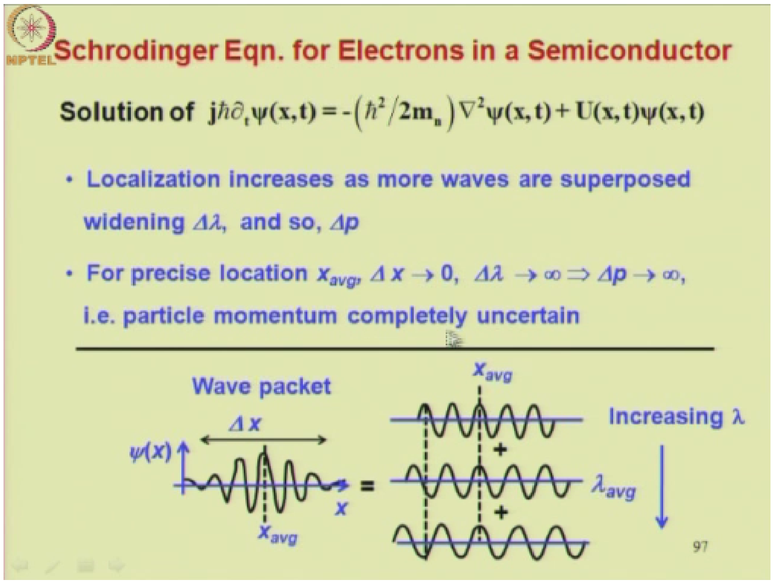

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Solution of $j\hbar\partial_t\psi(x,t) = -\left(\hbar^2/2m_n\right)\nabla^2\psi(x,t) + U(x,t)\psi(x,t)$

- Localization increases as more waves are superposed widening $\Delta\lambda$, and so, Δp
- For precise location x_{avg}, $\Delta x \rightarrow 0$, $\Delta\lambda \rightarrow \infty \Rightarrow \Delta p \rightarrow \infty$, i.e. particle momentum completely uncertain

So, localization increases as more waves are superimposed widening the uncertainty delta lambda and so delta p and taking the limit for precise location x average delta x should tend to 0, and this is only possible if delta lambda tends to infinity because you have a add infinite number of waves resulting in delta p to infinity. That is a particle whose momentum is completely uncertain.

So you are getting other result that if you try to locate the particle very precisely its momentum is uncertain. Earlier we showed if you have a particle with a precisely momentum then its location is uncertain that is this case. Now, that is the problem if you take the wave approach we are not able to simultaneously specify the position and momentum of the particle. And therefore a simple formula that we used based on classical mechanics which help you to derive the carrier concentration and momentum from the locations.

And the momenta of the various particles that cannot be used.

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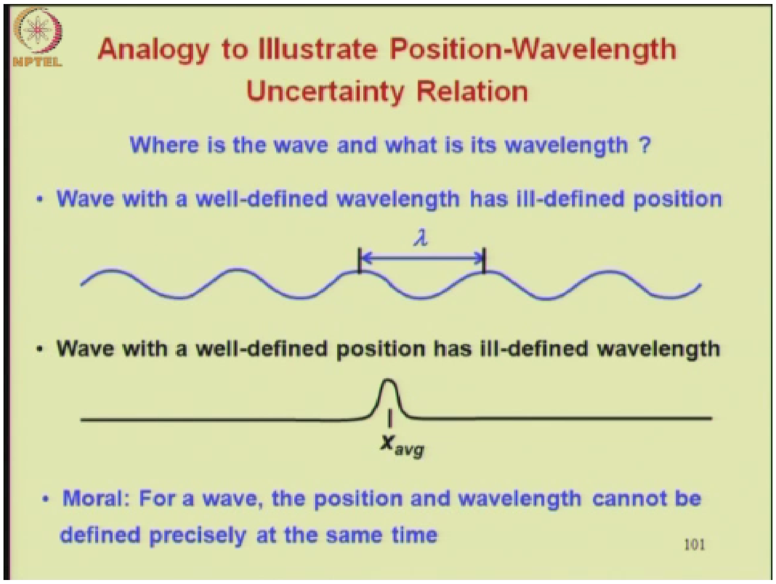

Analogy to Illustrate Position-Wavelength Uncertainty Relation

Where is the wave and what is its wavelength ?

- Wave with a well-defined wavelength has ill-defined position

- Wave with a well-defined position has ill-defined wavelength

- Moral: For a wave, the position and wavelength cannot be defined precisely at the same time

Now since this is an important point that you cannot specify the momentum and position of a particle precisely when you regard the electron as a wave this is a very fundamental result. So, let us make ourselves comfortable with this result with the help of an analogy. Let us take a practical case and ask the question where is the wave and what is its wavelength? Suppose you can show a wave like this which has a well define wavelength.

So, if you look at the wave you can definitely identify its wavelength. However, if somebody is going to ask you the question where is the wave? What is its location? Now, you know that you really cannot locate the wave precisely. It seems to be going everywhere. It exists everywhere. So, this is an example where if you know the wavelength precisely you can tell the location. Let us take the other extreme.

Now, this is a wave whose location you can specify with fair amount of certainty. Somebody ask you the question where is the wave? You can say, yes it is here. We will associate the location with the peak. Now if somebody is going to ask you but what is its wavelength? Well, you find no wavelength of this wave. So, it has an ill define wavelength. So, you see if you know of a wave which can be located precisely you really cannot associate a wavelength with it.

You cannot identify any wavelength. So, the moral is for a wave the position and wavelength both cannot be defined precisely at the same time. Now let us transfer this conclusion to our practical case of our practical problem of getting the carrier concentration and the current density of an electron from the wave view point.

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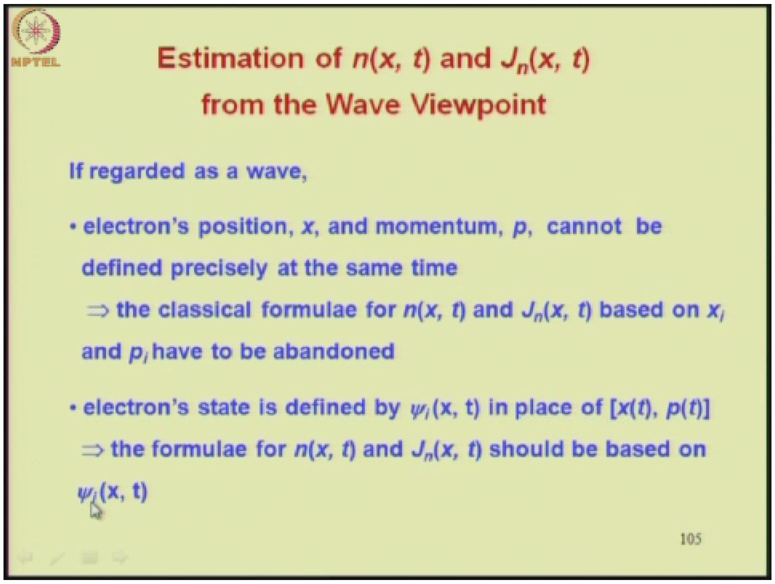

Estimation of $n(x, t)$ and $J_n(x, t)$ from the Wave Viewpoint

If regarded as a wave,

- electron's position, x, and momentum, p, cannot be defined precisely at the same time
  $\Rightarrow$ the classical formulae for $n(x, t)$ and $J_n(x, t)$ based on x_i and p_i have to be abandoned
- electron's state is defined by $\psi_i(x, t)$ in place of $[x(t), p(t)]$
  $\Rightarrow$ the formulae for $n(x, t)$ and $J_n(x, t)$ should be based on $\psi_i(x, t)$

So, if regarded as a wave electron position x and momentum p cannot be defined precisely at the same time therefore the classical formulae for n(x, t) and Jn(x, t) based on xi and pi have to be abandoned. Xi is the positon of i electron at an instant of time and pi is the momentum of the electron of the same electron at the same instant of time. Now, if regarded as a wave electron state is defined by psi i(x, t).

One function which has both time and distance variable in place of 2 quantities the location as a function of time and momentum as a function of time and therefore the formula for n(x, t) and Jn (x, t) should be based on the psi i(x, t) that is the wave function of the individual electrons.

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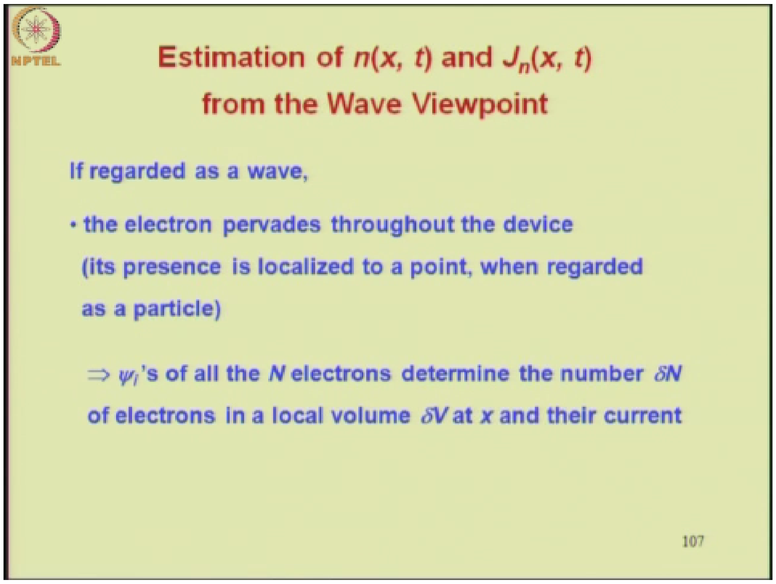

Estimation of $n(x, t)$ and $J_n(x, t)$ from the Wave Viewpoint

If regarded as a wave,

- the electron pervades throughout the device (its presence is localized to a point, when regarded as a particle)

  $\Rightarrow$ ψ_i's of all the N electrons determine the number δN of electrons in a local volume δV at x and their current

Further, if regarded as a wave electron pervades throughout the device. On the other hand, its presence is localized to a point when regarded as a particle. You see this is a very interesting information that we get if regarded as a wave right. It pervades all over even in the case you can see here when you are trying to improve the location of the electron you have the wave existing allover. Its amplitude is less no doubt.

The probability of finding electron else is small but it is not 0 that is the point. So, it exists everywhere therefore the wave functions of all the n electrons psi i of all the N electrons determine the number delta n of electron in a local volume delta v at x and the current due to these delta N electrons. So, you will recall when we did the current and carrier concentration modeling based on Newton's Laws we divide the device into local volumes. So we did something like this.

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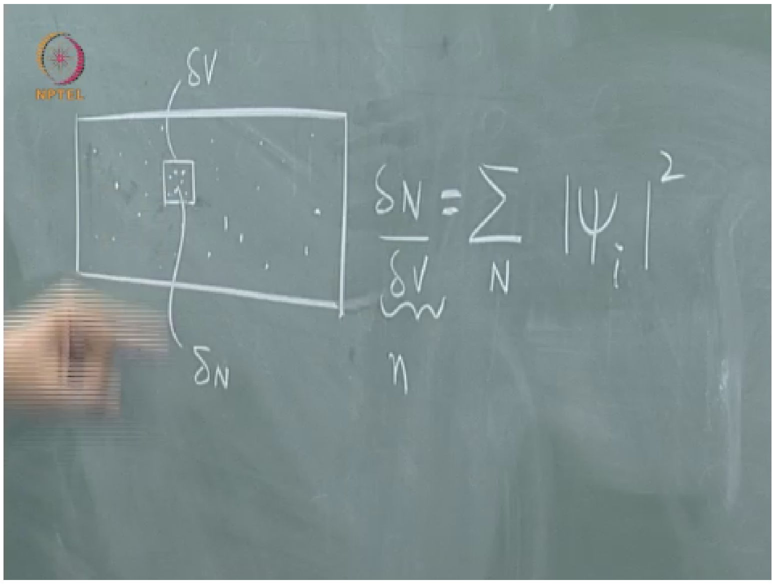

So, we said this is the device in which you have n electrons and then we took a local volume delta v and then we counted how many electrons here out of this n. So, this statement is regarding this situation. So the wave functions of all the N electron will determine delta N. Now from the wave approach if you want to find out what delta N here. The wave function of each of these electrons will also have to be taken into account.

Because from the wave point of view each of these electrons pervades allover though its probability may be very high at some locations but it is not 0 at other locations. So, even if I want to know how many electrons are here I should consider the wave functions of these other electrons.

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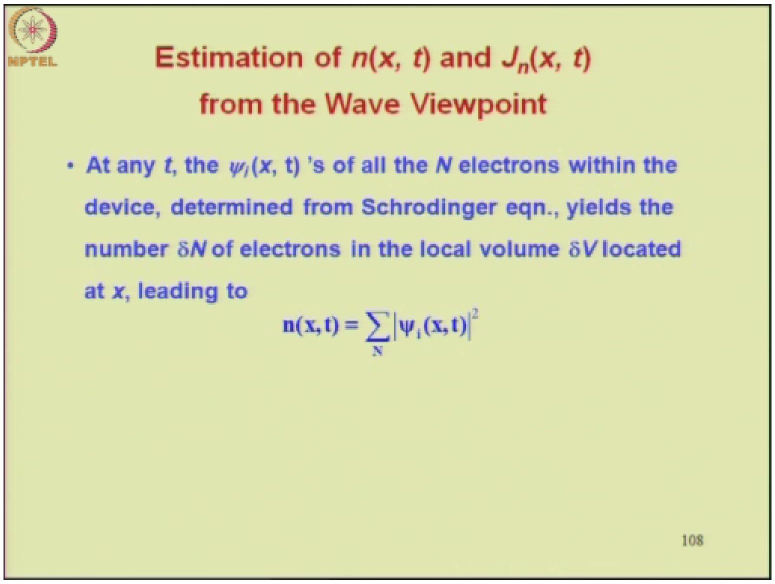

Estimation of $n(x, t)$ and $J_n(x, t)$ from the Wave Viewpoint

- At any t, the $\psi_i(x, t)$'s of all the N electrons within the device, determined from Schrodinger eqn., yields the number δN of electrons in the local volume δV located at x, leading to

$$n(x,t) = \sum_N |\psi_i(x,t)|^2$$

Therefore, we can set out the procedure as follows at any t, the psi i (x, t) of all the n electrons within the device determine from the Schrodinger equation yields the number delta N of electrons in the local volume delta V located at x, leading to this formula. n (x, t) = psi i (x, t) square for all the n electrons sum together. Now, this formula can be derived very simply as follows.

So, concentrate on this volume delta v now take the wave function of each of these electrons that is psi i square it, integrate it over the delta v that gives you the probability of finding the i th electron in this volume. So, i is the wave function of i-th electron so when integrate over this I get the probability of finding this electron in this volume like that I should do for all the electrons. All the n electrons so that is how you get here. Then what will you get?

Then you will get this number delta n so the number of electrons here is delta n so you will delta n here. So, if I now put this delta v here this ratio delta n/delta v is nothing but your n carrier concentration within this local volume wherever you are located it. Let us say I located at some x here so that is the result.

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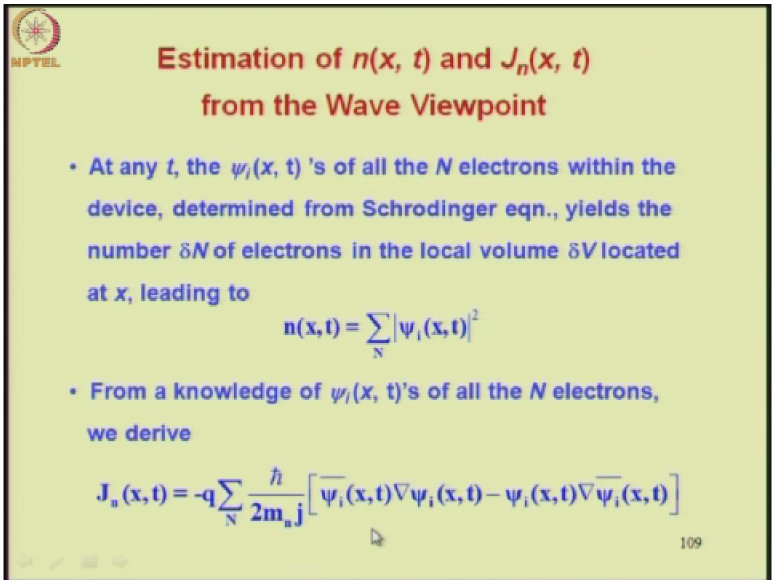

Estimation of $n(x, t)$ and $J_n(x, t)$ from the Wave Viewpoint

- At any t, the $\psi_i(x, t)$'s of all the N electrons within the device, determined from Schrodinger eqn., yields the number δN of electrons in the local volume δV located at x, leading to

$$n(x,t) = \sum_N |\psi_i(x,t)|^2$$

- From a knowledge of $\psi_i(x, t)$'s of all the N electrons, we derive

$$J_n(x,t) = -q\sum_N \frac{\hbar}{2m_n j}\left[\overline{\psi_i}(x,t)\nabla\psi_i(x,t) - \psi_i(x,t)\nabla\overline{\psi_i}(x,t)\right]$$

Let us look at the result for the current. From knowledge of psi I (x, t)'s of all the electrons we derived the current expressions as follows. Now let us explain this current express. How do you get? We can link it to the expression based on the classical approach, based on Newton Law approach. In the classical approach if you recall your current expression was as follows.

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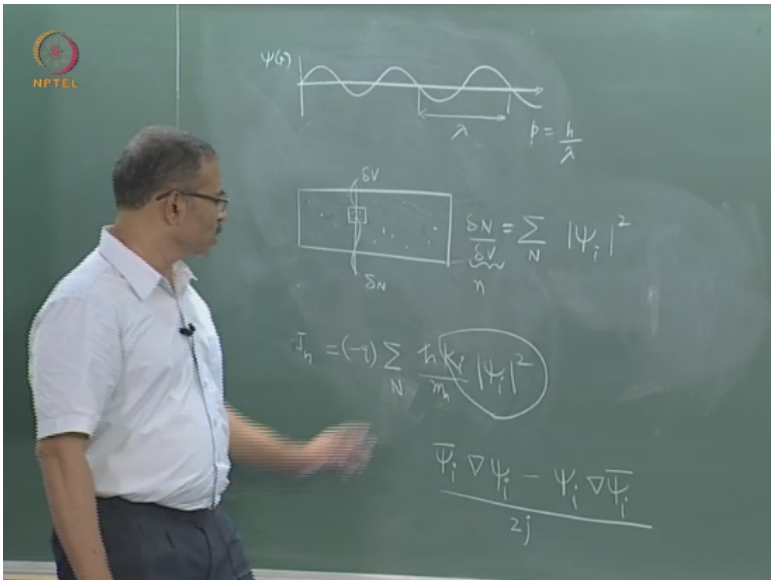

Jn was because of this delta n electron. So you found out the find out the momentum of each of these electrons within the local volume that is Pi you divide it by the effective mass and sum up for all the delta n electrons then multiply it by -q that gives you the current density. Now suppose you extract the approach to the wave point of view. Now you know that from the wave point of view the momentum pi can be expressed as h cross times Ki where Ki is the wave vector for the i-th electron obtained from the wave function.

So look at this wave function here. This is the k square and this is the k. So for the i-th electron you must find out what is this k? What is the energy? depends on the energy. So, h of Ki now however as we said the wave pervades everywhere so I must choose all the n electrons. Now, the probability that i-th electron will be in the local volume delta v is probability psi i square and so I should do this for all the n electrons.

So, you see what is happening is when I move from the classical picture to the quantum picture the delta N is getting replaced by all the N electrons but what is coming here is the probability density of finding the i-th electron in that location. Now, it turns out that this simple approach that we have adopted corresponds to the case of a plane wave that is the wave like this. But you know that in practice supposing you are talking about locating a particle.

Then you will have a probability distribution function like this. In other words, you can have a wave packet. So you can have different types of wave functions so you need a more general result that is applicable to other cases as well. It turns out that more generally this quantity works out to –we are not going to do a detailed derivation here but we will only explain the result. This quantity works out to the conjugate of psi i multiplied by the gradient of psi i - psi i into gradient of the conjugate of psi/2 times j.

So, this j is coming because when you do this exercise you will have the numerator complex so you are dividing it by j to make it real. And then there are 2 terms here both of them contribute and therefore you divide it by 2 to get this kind of relation. Now, how to explain this kind of an expression here now you know that we have said earlier that the current is the probability current.

So, electrons are moving from one point to other point because the probability of finding an electron at one point is higher than the probability of finding an electron at other point. Therefore, the current depends on the gradient of the probability that is what is coming here actually that is why you have gradient terms here. So, because of this there is a momentum generated because there is a probability gradient there is the driving force for motion and a momentum is generated.

That is how this is coming into picture here. So, this can explain the form of the equation that you see here for the current density.

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Summary of this lecture

Now we come to the end of the lecture therefore let us make a summary of the important points. Now, this entire lecture was devoted to finding out the carrier concentration and current density from the state of the individual electrons as determined from Schrodinger equation. So, we essentially discuss the individual carrier view point regarding the electron as a wave. So, first we explain how the Schrodinger equation looks like for a semiconductor crystal?

What are the various potentials that the electrons are subjected to then we discuss the solution of this Schrodinger equation for a very simple case and we showed that because of the difficulty of specifying the location and momentum of an electron simultaneously and precisely. The formula for carrier concentration and current density becomes more sophisticated, a little bit more complex than the case of classical mechanics.

“Professor - student conversation starts” Sir, I have a question can you clarify once again how j comes on the left hand side of the Schrodinger equation and -1 comes as the coefficient of the square term.

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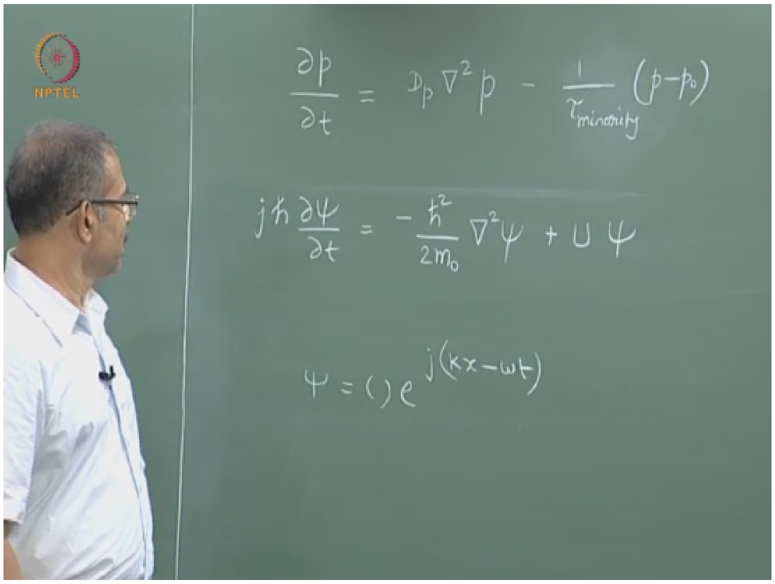

$$\frac{\partial p}{\partial t} = D_p \nabla^2 p - \frac{1}{\tau_{minority}}(p - p_0)$$

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

$$\psi = (\ )e^{j(kx - \omega t)}$$

So, your doubt is related to this equation here. How j arises here and why -1 term comes here when you see the correspondence of this equation to this equation here you do not have any j or anything like that and here the coefficient is positive. So, let me clarify that we are not discussing here the derivation of this equation but we are trying to explain how we can more ourselves comfortable with the form of this equation so that we remember it for long time. “Professor - student conversation ends”

Now, the way to understand it is very simple since psi is the solution of wave equation psi is a travelling wave. Now you know that a travelling wave always has a coefficient like this so into something so psi= something into this. So, here you see kx - omega t now one may discuss about the sign here should it be -/+ and should this sign be here +/-. We will not get into that discussion right now.

Let us just use this form which we are very comfortable with which we have used in our earlier courses and explained how this sign arise here and how this j arises. Now, ones you assume a form like this clearly when I differentiate psi with respect to t, I will get a -j out. There is a negative sign here and there is j. So, I will get -j out but ultimately the coefficient of the term here when you differentiate you will get psi itself multiplied by a -j term.

So, the coefficient of psi you can see here this quantity is real. So, everywhere after you perform the operation indicated here look at the whole term it should come out as some coefficient into psi that coefficient should correspond to the coefficient shown here. For example, the coefficient here should be positive. You can see that the coefficient of the delta square term here is positive and similarly the coefficient of the term psi, term here should also be positive as shown here.

So, now you can easily see that by differentiating with respect of time if I am going to get a -j out to make the coefficient +1, I have to multiply -j/j then -j square would become +1. Similarly, if I differentiate with respect to x twice which is what this ask you to do. So, take this and differentiate twice I will get once j with one differentiate. Second differentiate will give me again another j.

So, I will get j square out and j square is negative where as I want the coefficient to be positive as shown here if it is in a delta square form. Therefore, I multiply the term by -1 so that this -1 multiplied by the -1 coming out of this operation makes it +1. Sir, can you similarly clarify the sign of the third term U psi term? Your doubt is that you that here you see a negative sign as coefficient of the p term which is the p term here.

Similarly, your doubt is why should the coefficient of this term here be positive whereas here it appears to be negative? Well, as we have discussed earlier that this term is a source or a sink term. For example, p - p0 here could be positive or negative thus after a negative sign is attached to this, this whole term could be positive or negative. It turns out that here this term is written as a positive term. It is +U into psi and it is a source term actually.

It gives rise to probability it is not a sink term it is a source term.