Semiconductor Device Modelling and Simulation
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Lecture – 57
Quantum Transport

Hello, welcome to lecture number 57. We will continue our discussion on Quantum Transport. So far, we have discussed about postulates that are used in quantum mechanics. Then the Schrodinger equation how to solve the Schrodinger equation? And it leads to the quantization and the localization of the states. And then we also discuss the quantum correction models that are prevalent.

Now, in today's lecture we will further continue our discussion on quantum transport. So, specifically, we will consider one example how to calculate the carrier concentration in a quantum band? Then the quantum transport through a potential step how far electron can penetrate inside and tunneling through a potential barrier.

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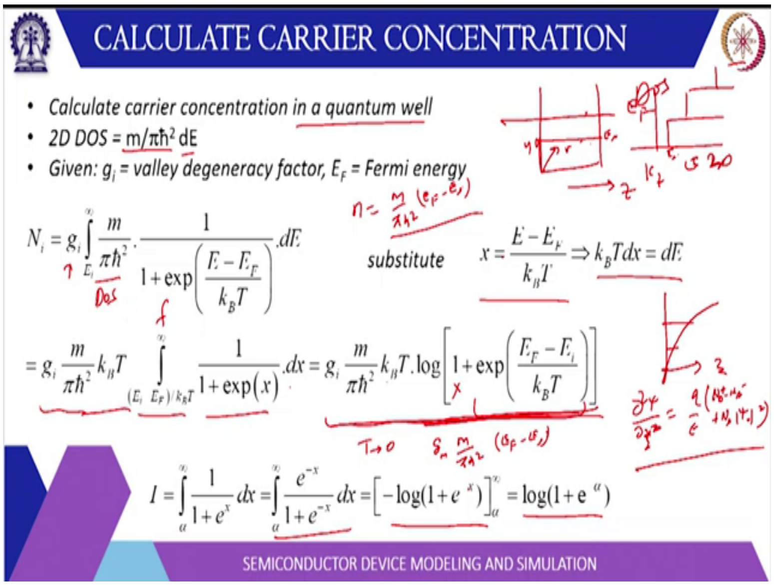

So, let us calculate the carrier concentration in a quantum well. So, as you know that quantum well is a kind of it is constrained in 1 dimension. Let us say this is the z dimension and in x and y direction it is free. So, there will be the z direction that means the k z will be quantized and k x and k y can take any arbitrary value. Now, if you recall, we calculate the density of a state for 2D system and it was m by pi h bar square.

In energy step D this is the number of states and this is basically constant. So, once you encounter a state here then beyond this let us say this is the energy level of density state then beyond this the density of state is fixed. So that is how we got something like this. So, this was a DOS for 2D structure versus energy. Now, let us say Fermi level somewhere above this E i.

Let us say Fermi level somewhere here, here so, up to E i to E F this will be occupied. Now, at 0 kelvin it is fairly simple that up to E F it is occupied. So, you can easily say the number of carriers will be m by h bar square times E F – E i, E i is the energy level of that particular state. But if you consider any arbitrary temperature, where Fermi direct distribution is followed by the electrons.

So, it is no longer a step profile then of course you have to multiply the density of a state m by pi h bar square times the Fermi track distribution function that integrate from the energy level. Because after this E i it is non-zero below this it is 0 so, from E i to infinity. And g i is basically valley degeneracy factor that is how many such valleys are there, where this density of state exists basically.

So, this is a simple integration that can be solved by making a substitution. Let us substitute x = E – E F by k T. So, the denominator becomes 1 + exponential x this is a constant, so, can be taken out. So, g i times m by pi h bar square. Then from this you can say that dx = dE by k T or d can be substituted as k T times dx. So, it is k T times g x k T again constant, so, it is taken out.

And limit you can modify because initially it is E i to infinity. So, if you substitute E i then x becomes E i – E F by k T. So, this is a lower limit infinity if E is infinity x will also infinity, so, it is from this E i – E by k T to infinity. Then this is a integration that you can easily solve. What you have to do, basically? You multiply numerate and denominator by e to the power –x so, it is shown here. Let us say this is some limit alpha to infinity.

Then it is e to the power –x dx by 1 + e to the power –x and it is integral is log of 1 + e to the power –x with a minus sign and then at infinity this will become 0, so, log of 1 is 0. Then only you have to calculate it at alpha and alpha is minus, minus cancel out so, log of 1 + e to the power –alpha so that is shown here 1 + exponential E F – E i by k T. So, this is required because if you recall this quantum correction model.

Especially, at the MOS structure where these quantized states, so, we have to calculate these energies this carrier concentration in the quantum wells. So, when you write the poisson equation that is del 2 e by del 2 psi by del x square is q by epsilon. So, let us write del 2 psi by del x square or z square in this case, you cannot z square if this x direction is z. Then is equal to q the charge on electron times the total charge.

So, in this region there will be impurity concentration. So, let us say that is N D +– N A minus and then plus the concentration of electron. So, this is basically the carrier concentration. So, you can write N i and then psi i square divided by epsilon. So, this calculation is required in the case of quantum correction model. So, I just took one example similar way you can calculate the carrier concentration for 1D, 2D, 3D profiles.

For 3D also we can get expression but if you recall for 3D density of a state when we calculated, we got Fermi track integral. And then when it is non-degenerate semiconductor that means Fermi level are sufficiently away from the band edges. Then you could get nice expression e to the power e – E F by k T that expression you could get. But in case of 2D it is log of 1 + exponential E F – by k T.

And you can also see if T 10 to 0 then this basically exponential 1 by 0 basically this will be large. So, you can ignore one so, log of exponential release, simply E F – E i by k T and this k T will cancel out. So, you will have g i times m by pi h bar square times E F – E i at 0 kelvin. So that is what we you know approximated without the calculation also.

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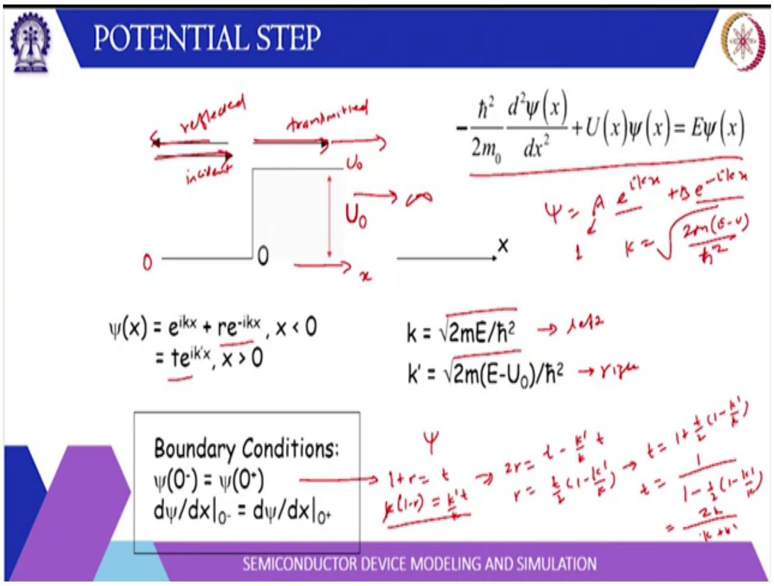

So, let us continue now let us understand how the electron wave function will respond when it encounter or it goes through a potential profile. So, let us consider simple case there is a potential step. So, let us say potential is 0 here and potential is U naught here. Now, let us say some incident wave is falling on this barrier then some will get transmitted and some will get reflected. So, this is incident, this is transmitted and this is reflected.

Now, if you recall the Schrodinger equation, you can always write psi = sum A e to the power iota kx + B e to the power – iota kx and where k is root of 2m E – U by h bar square. So, for left side you can write because U is 0. So, for this is for left side root 2mU h bar square right side U is U naught. So, for right side you can write root 2m E – U naught by h bar square, where e is the energy of electron and U is the potential.

Now, if you see here, there are two terms here plus iota kx – iota kx so, plus iota kx is forward traveling or the incident wave minus iota kx is the reflected wave or –x direction traveling. Now, for the transmitted wave, we have only considered one because we assume that this is infinite, so, there is no more reflection. So, whatever is transmitted will go ahead basically.

So, at the interface we can see one way of transmitting to the point along the positive x direction and two waves in the left region one is travelling to +x direction, other travelling into –x direction. So, we can use A and B or you can normalize it let us say assume that this is one. So, you can write B will become basically the reflection coefficient and t will become the transmission coefficient.

So because for the reflection and transmission anyway they are calculated with respect to the incident wave in a general case, you can normalize it to one basically. So, either you write a + b or you write e to the power iota kx + re to the power – iota kx. It does not really matter. Now, let us apply the boundary condition. So, if you recall that psi is a wave function which is single valued which is continuous and it is derivative is also continuous.

So that means your psi has to be equal at 0 + and 0 –. So, 0 minus this is basically 1 + r at 0 + this is t. So, this tells you basically, 1 + r = t. Thus one condition if you take the derivative d psi by dx so, this will become k times e to the power iota kx. This become minus kr, so, k into 1 – r e to the power iota kx at x = 0 is becomes 1 is equal to here the derivative k prime iota k prime, so, iota will cancel out, so, it is k prime t.

So, you will get these two equations and from this we can find the expression for r and t. So, r you can find easily what you can do? You can take this here, k prime by k. So, you can write if you subtract then 2r = t – k prime by k times t. So, this is your r basically, so, r is basically t by 2 1 – k prime by k. So, if you substitute this r here, you can get basically expression for t.

So, substitute in first equation so, you get t = 1 + r so, 1 + t by 2 1 – k prime by k. So, if you rearrange then you can get the expression 1 + 1 divided by 1 – 1 by 2 into 1 – k prime by k and that basically comes out to be 1 – 1 by 2 so, 2 can be taken out then this becomes 1 + k prime by k. So, k will be here and this will be k + k prime. So, you again, if you substitute it back here, you can get the expression for r.

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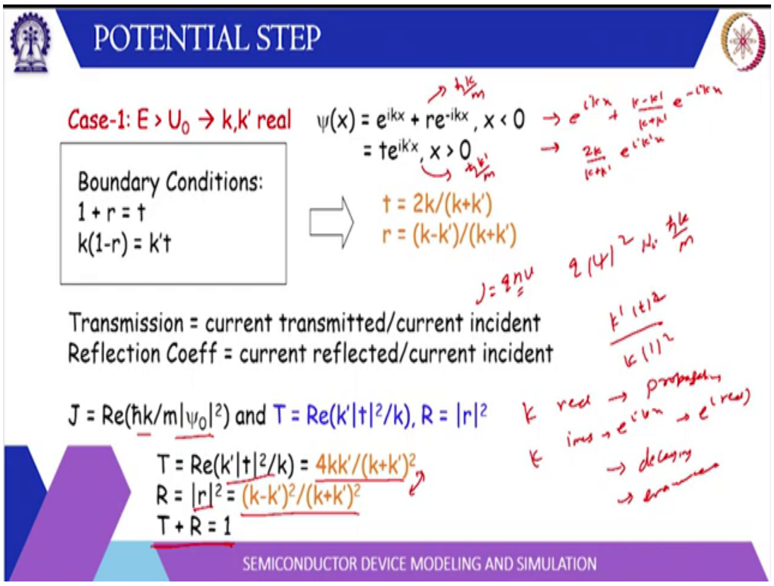

So, it is shown here the t is 2k by k + k prime and r = k – k prime by k + k prime. So, using you can write that your psi is basically e to the power iota kx + k – k prime by k + k prime e to the power –iota kx. And this is 2k by k + k prime e to the power iota k prime x. So, these are the wave functions basically. Now, the current is calculated in terms of the wave function. Wave function psi square tells you the density of carriers.

It tells you the carrier density this is one of the postulate. And if you want to calculate the current then if you recall the expression for current J = q times n times V. So, you can multiply this q and sigma square tells you about density, you can multiply by N i and so on and V is the velocity. So, V means the velocity is related to k. So, it is h bar k by m. So, for left side this region, the velocity h bar k by m, for right region it will be h bar k prime by m.

So, you notice here the reflection coefficient will be simply the ratio of r square because the reflected wave and the incident wave both have the same velocity that is h bar k by m. So, your R is simply magnitude of r square that is a reflection coefficient. Then the transmission of course it has to be multiplied by different k. Because transmitted one the velocity is k prime times t square and the reflected one is k primes that is 1 square.

So, it is k prime, by k times t square. And now, you have to take the real part because if t prime is imaginary, it means it is decaying basically. See if k is real that means the wave is propagating, if k is imaginary then e to the power iota kx is the e to the power the coefficient is real. And usually it is negative because you know otherwise the L is for the transmitted region it will go to infinity so, the psi has to be bounded also.

So that means this is a decaying wave or it is also has a name evanescent wave. So, it will be k prime, by k times t square, so that will be 4 kk prime by k + k prime whole square. Now, if you add these two terms, you should get one because incident current is equal to reflected current plus transmitted current. So, the reflection coefficient plus transmission coefficient should be equal to 1.

Now, you note here this is basically the current, not the magnitude of the wave function. So, it is the k times the psi square. Now, if energy of the electron is less than the potential barrier. So, first case was energy was more than the barrier energy so, we found these values basically.

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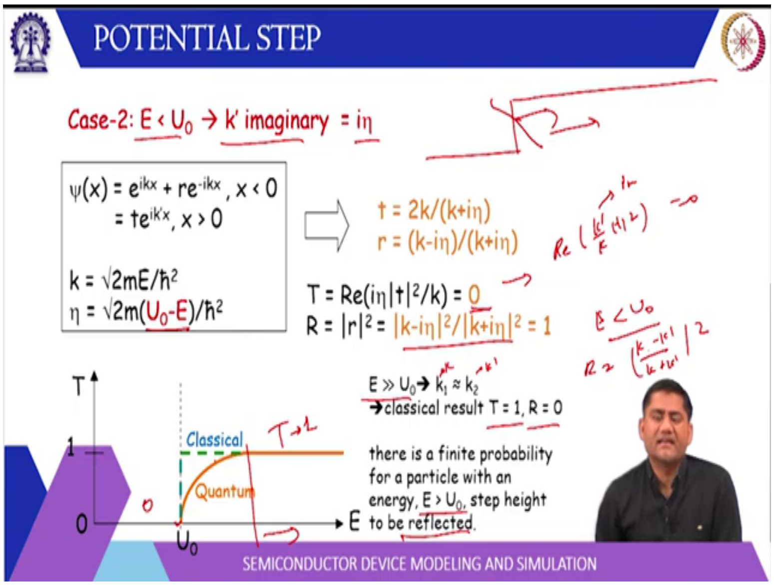

If energy is less than U naught then k prime will be imaginary. So, you can write k prime is iota times some number eta. And then eta can be written as you reverse the order instead of E – U naught you can write E U naught – E so that it is positive because now E is less than U naught. Then if you look here the transmission coefficient which was real part of k prime by k times t square. Now, k prime is imaginary, so, this is imaginary, so, the real part will be 0.

So that means there is no transmission. So that means when energy of the electron is less than U naught, there is no transmission. It is same as the classical case. Now, this is for potential barrier that means this is potential barrier which is infinitely thick. So, there is a potential vary which is infinite to the extent. So, in this case there is no transmission, it does not mean there is no penetration, the wave function may penetrate but it cannot propagate.

And of course, if t is 0 then reflection coefficient has to be 1. So because this is your reflection coefficient is k – k prime by k + k prime whole square. So, this is k prime is imaginary so, it is a complex number. So, they are obviously complex conjugate of feature and that will always be 1. So that means the reflection coefficient is always 1 and the transmission coefficient is always 0 when energy is less than U naught.

But if energy is more than U naught then transmission is not always 1 that you can see from this one. So, both are basically non-zero when energy is more than U naught. Now, you can write a simple Matlab code to plot it. So that means there is a finite probability for a particle with energy more than the potential barrier to be reflected. Now, classically this was not the case that electron can basically.

If it is energy is more than the barrier height it will just go through. But in quantum case this is not the case that electron can still be reflected. Now, of course, you can estimate it if energy is much larger than the potential barrier height then the k and k prime, let us say this is k and this is k prime, they will roughly be equal. Because now this, U naught is very small, so that means t will be now close to 1.

So, for energy which has very high this T is 1. For energy less than U naught the t is 0 and in between there is a transition. So, you can understand this fact that at a potential barrier if the energy of electron is less than the barrier height, it will always be reflected there will not be any transmission. Although, there can be a penetration of the wave function. If energy is more than the barrier height then there is a finite probability that electron can still be reflected.

And if energy is much higher than the barrier height then it is same as the classical case that this electron will always get transmitted.

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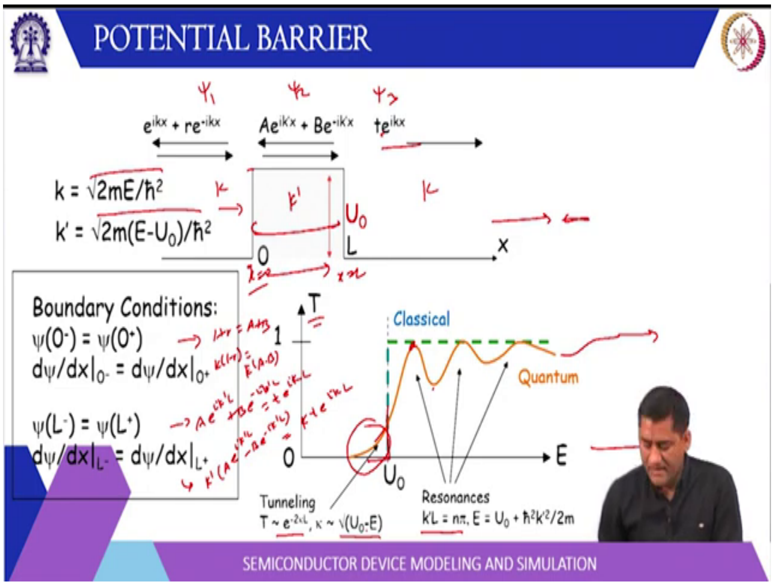

Now, let us restrict the thickness of this barrier. So now, although height is still U naught but now length is not infinite it is 0 to L. So now, we will have two boundary condition one at x = 0 other at x = L. Now, you can notice one more thing here in this region this is k, this is k prime and this is again k. Because here also U is 0, so, in case root 2mE by h bar square and k prime is root 2m E – U naught by h bar square.

Then of course you can write this is transmitted wave so because this is infinite to the extent. So, there is no reflection here, so, you can write t times e to the power iota kx. This is e to the power iota kx plus reflection, e to the power –iota kx. And in this region let us write A times e to the power iota k prime x + B times e to the power –iota k prime x. Then of course we will again apply the boundary condition.

So, this is your psi 1, this is psi 2 and this is psi 3 so, at x = 0 psi 1 and psi 2 they should be continuous their derivative should be continuous. So that gives you the condition at 0 + and 0 – so, 1 + r = A + B and if you take the derivative then k times 1 – r = k primes times A – B. At L A times e to the power iota k prime L + B e to the power –iota k prime L = t e to the power iota kL.

And if you take the derivative then this will be k prime times A e to the power iota k prime L – B e to the power –iota k prime L = k times t times e to the power iota kL. So, these are the four equations you will get and then the characteristic that you will get is very interesting. Now, in this case, when energy of the electron is less than the barrier then there is a finite probability of getting it transmitted.

That means, even though the energy of electron is less than the barrier height. There is a finite probability that it can get transmitted. So, this x axis energy, energy is less than U naught and then the transmission probability is finite here. And of course it increases it goes to a peak. Then of course it does not stay there it comes down and approaches classical limit of one. And of course, at high energy this will be actually exactly one.

So, in between some kind of this resonance thing we are finding out. This is due to the this barrier basically. So, when barrier is certain wavelength long, there is a high probability that this will be one and if it is opposite then the transmission will be less. So, these are the basically resonance points and they correspond to k prime L = n pi. So, this length is order of half wavelength multiple of half wavelength.

And this region is called the tunneling, so, tunneling is e to the power –2 kL and k is root of proportional to root of U naught – E let us drive it.

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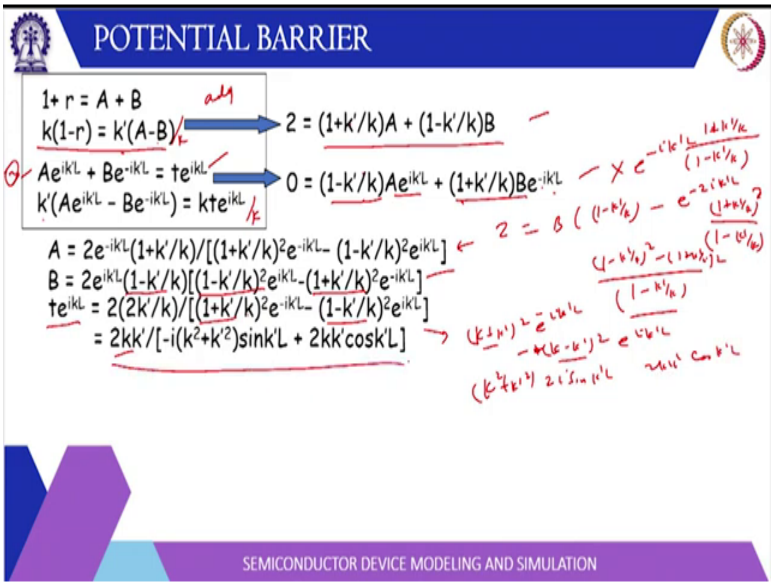

These are the four boundary conditions. We got two equations 1 + r = A + B k times 1 – r = k prime A – B. And if you divide second equation by k and add so on left side, you will get two on right side A times 1 + k prime by k and + B times 1 – k prime by k. So, this is one equation containing A and B. So, we have eliminated r here, in second equation also, you can eliminate t.

So, how can you limit t? You divide this thing by k and subtract, so, this will be 0, so, this is 0 and this side you have A times e to the power iota k prime L and this is 1 – k prime by k. Similarly, + B e to the power –iota k prime L times 1 because we are subtracting, so, it becomes 1 + k prime by k. Now, we have two equation in terms of A and B and we can solve it to find the expression for A and B.

And we know A and B then we can find t also we can substitute here and get the expression for t. So, by solving these equations these are also simple, how can you do it, basically? If you look at these two equations less eliminate one of them. So, how will you eliminate? So, what you can do? You can multiply this by e to the power –iota k prime L and 1 – k prime by k in the denominator and 1 + k prime by k in the numerator.

So, these two will be equal basically then you subtract. So, on left side you will get 2 is equal to this will go to 0 and then you can have B here this is 1 – k prime by k then – e to the power iota kL, iota kL is multiplied, so, it is e to the power –2 iota kL – 2 iota k prime L. Then 1 + k prime by k whole square divided by 1 – k prime by k. So, if you rearrange it, you will get the expression for B because this will be multiplied.

So, you will get B is equal to e to the power 2 times so, cancel out. This is what so this is here it becomes plus here. So, 2 times e to the power iota kL and then this, if you normalize then you have 1 – k prime by k and numerator you have 1 – k prime by k whole square – 1 + k prime by k whole square. So, you will have 1 – k prime by k whole square, 1 + k prime by k whole square and 1 – k prime by k here in the multiplication.

And 2 one of them is written here because this is e to the power –iota kL. So, you will get basically this expression **(()) (26:22)** little algebra and similarly by eliminating B you can get the expression for A. And when you substitute the value of A and B in this third equation you can get the t times e to the power iota kL. So, this is 2 times 2 k prime by k times 1 + k prime by k whole square e to the power –iota k prime L – 1 – k prime by k whole square e to the power iota k prime L.

Now, if you see here again you can rearrange it k you can take out. So, it is k + k prime is whole square it is k – k prime whole square. So, this is basically k + k prime whole square e to the power iota k prime L – then – k – k prime whole square e to the power iota k prime L and then this k square goes up, so, it will become 2k times k prime. Now, this is written as k square + k prime square + 2 kk prime and then this is k square + k prime square – 2 kk, prime L.

So, you can write, k square + k prime square and then subtraction e to the power –iota kL – e to the power iota kL. So, this becomes 2 iota sin k prime L and this is 2 kk prime 2 kk prime this become positive, so, 2 kk prime will have cos k prime L. So that is what you get the denominator.

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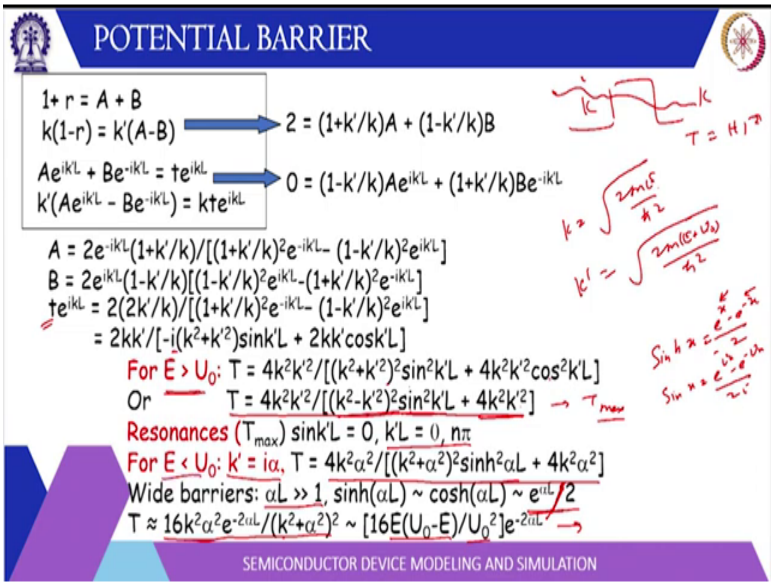

Now, this can be further analyzed for energy more than U naught. So, just recall what is k? K is equal to root 2mE by h bar square and k prime is root 2mE – U naught by h bar square. So, this is remember this is t small t, so, capital T can be found out. In this case, this is also k, this is also k so, your capital T will be small t square basically. Because now both are k basically, so, this will be simply capital T square.

So, this will be the expression k square k prime square whole square sin square k prime L + k square k prime square cos square k prime L. So, if you put them together, you can write it as whole square and then this becomes cos square + sin square. So, this becomes 1so, 4k square k prime square. Now, if you notice here this is the final expression for the transmission coefficient.

Here we have only one sin term and this will be maximum that means t will be maximum if this goes to 0 and sin k prime L will be 0 when k prime L is n pi or 0. So, this is for E less than E more than U naught if E is less than U naught then k prime is some iota times some number because k prime is now complex. So that means what will happen? This will decay this is going this is decaying and then transmitting basically.

So, it depends on the length and the height of the barrier. So, if you replace k prime by some imaginary number out alpha. So, the expression becomes 4k square alpha square by this thing and sin k prime L is sin iota alpha L and sin of imaginary number is called sin hyperbolic. And if you recall sin hyperbolic, let us say some number x is e to the power x – e to the power –x by 2.

And this is if you write sin x it is e to the power iota x – e to the power –iota x divided by 2 iota. So, this is basically because this is iota times sin k n so, it becomes sin hyperbolic alpha L basically. Then here also so, you can see for wide barriers alpha L or L is much larger than 1 so, sin hyperbolic and L or the cos hyperbolical they will be e to the power alpha L whole thing divided by 2.

Because this x is large, so, e to the power –x can be neglected. So, it is e to the power x by 2 so, this is e to the power x by 2. So, it is not alpha L by 2 which is e to the power alpha L whole thing divided by 2. Then if you substitute here then you get this expresses 16 k square alpha square e to the power –2 alpha L by k square + alpha square whole square. And kl square alpha square you can see, k is proportional to E alpha square is proportional to U naught – e.

So, it is E times U naught – E divided by U naught square because k square + alpha square will be U naught square e to the power –2 alpha L. So, this is the expression for the tunneling for energy less than the barrier height.

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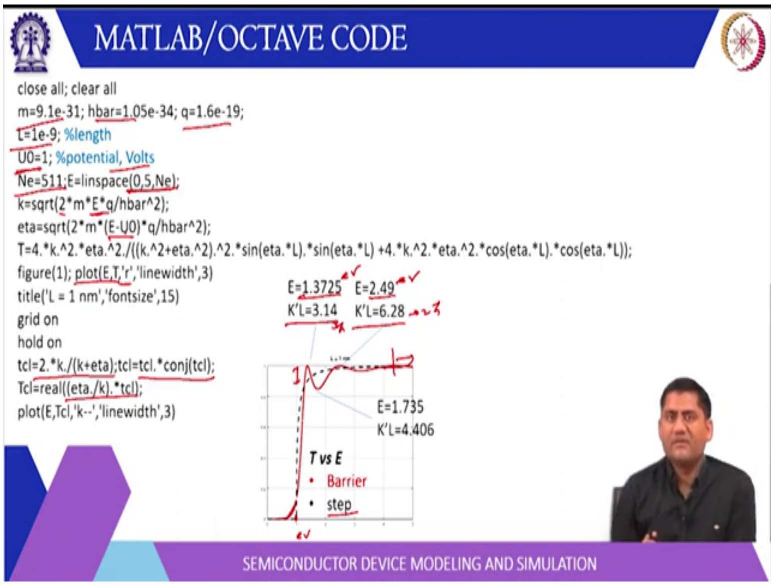

Now, you can write a simple Matlab code that I have done here. So, this is the mass of electron then h bar q the length is taken as let us say, 1 nanometre U naught is 1 unit is electron volt. So, what you will write here? We will multiply it by q so that is electron volt then number of steps 0 to 5 volt potential is taken, energy is taken and there are 511 elements are taken. Then case root 2mE by h bar square, so, energy is assuming electron volts.

So, we are multiplying this by q basically, so, this energy is also 0 to 5 electron volt and potential is 1 electron volt. So, k is this eta is square root of 2mE – U naught by h bar square. So, this is same as alpha that I mentioned so r is it k prime basically, it is k prime E – U naught so, it is k prime opposite of this will be eta. So that means when energy is less than U naught this will be imaginary for energy more than U naught this will be real.

Then transmission is 4 k square eta square this expression is written here. Then we are plotting this transmission versus energy. So, what you see here? This is a red curve basically is a r, r is for red curve. So, red curve is a transmission and you can see that at this point where energy is 1.3725 if you can calculate k prime L it is comes around 3.14. So that k prime L is actually pi here is only at 2 pi at 2.49 energy electron volt.

The k prime L is 6.28 which is 2 pi so, this is 2 pi and this is pi. So, you see there is a resonance transmission here and it is start transmitting at energy less than the barrier height which is 1 electron volt. Now, simultaneously I have also plotted the for a step area where this per established 2 k by k + eta. So, what I do? I take a square of this so, multiply this by complex conjugate and take the real part eta by tcl.

So, this black curve is basically for the step and you see for energy less than U naught there is no transmission but for energy more than U naught or 1 electron volt it is not 100 percent transmission but it gradually reaches. At of course, high energy the transmission is always one regardless of the barrier height and the length.

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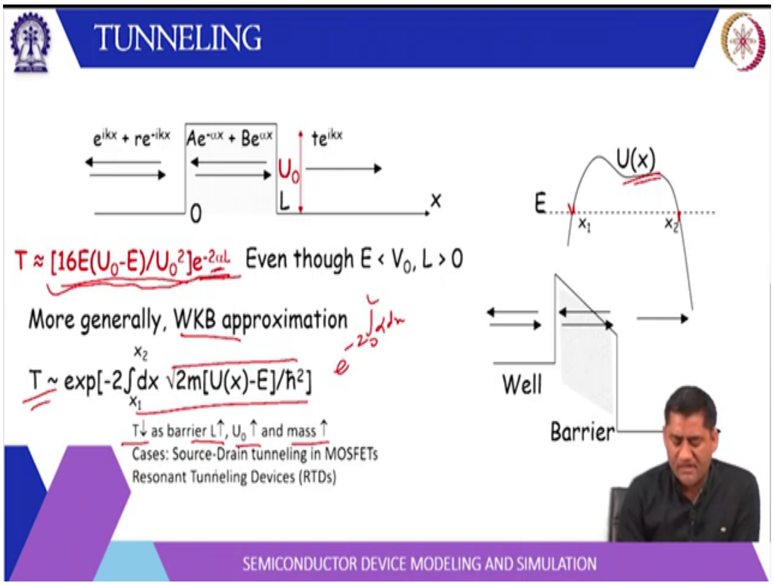

So, this understanding of the electron going through a potential barrier and the tunneling phenomena gives right to some kind of devices that they use the tunneling phenomena. So, since we have discussed this thing for a constant profile. Now, this principle can be applied to a general profile where potential is not constant, whether there is some function of position.

So, in that case, if you look at the expression, it is 16E U naught – E by U naught square times e to the power –2 alpha L. So, this can be roughly assumed to be constant and exponential being a dominant term. So, you can write e to the power –2 alpha L and alpha is root 2m U – E by h bar square. So, this alpha is basically function of position, so, you can integrate it or from this let us say this is x 1 to x 2.

So, integrate this thing then two times – 2 times this alpha dx, basically where alpha is a function of position. So, what you have written here, e to the power –2 alpha dx and this is 0 to L or x 1 to x 2. So, this is the transmission probability sand this approximation as a name, is called WKB approximation. It is named after scientist Wentzel, Kramers, and Brillouin so, probably known as WKB approximation.

And if so, you can notice from here that tunneling will decrease as the barrier thickness increases or the barrier height increases or the mass increases. So, this will reduce the tunneling and in MOSFET you can see the source to drain tunneling or you can also see the resonant tunneling devices.

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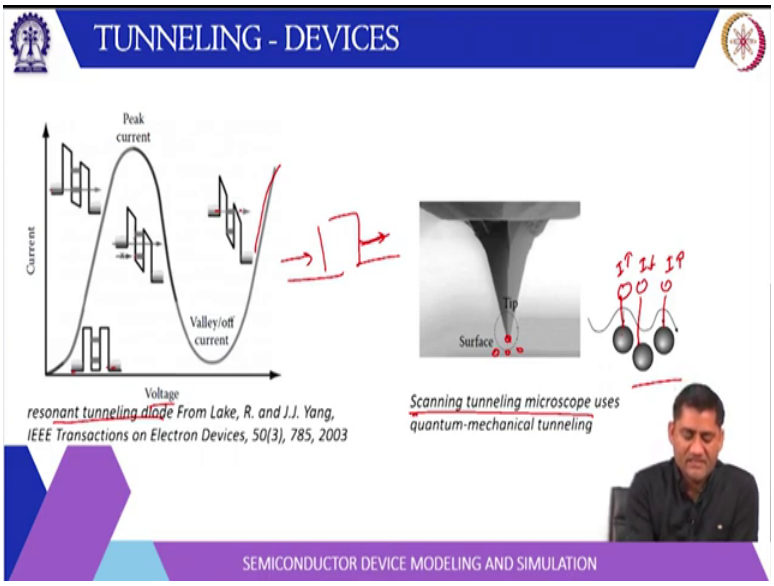

So, some devices that use this phenomena one is of course the resonant tunneling diodes. Other is the scanning tunneling microscope. So, there is a tip here which has also atoms here at the surface, there are atoms here. And they can measure the atomic distance because it is very sensitive to the barrier. So, this is basically barrier, so, there is a atom here and these are surface atoms, so, you see, this is a distance here, this is distance here.

So now, tunneling current will be more, more current here, less current here then more current here. So, this current profile actually gives you the surface profile. So, this is the principle of scanning tunneling microscope. It was invented in 1981 by Gerd Binnig and Heinrich and for this they also earned the Nobel Prize in physics in 1986. Now, for tunneling another thing that you might know the tunneling takes place when there is a state in between.

So, if there is no state then tunneling will reduce basically. So, you see here at the beginning, there is less tunneling then when there is a state here, a tunneling increases and then in between it decreases and then when another state comes here, it again increases basically. So, in between if there is a state because tunneling can take place, if there is a state for these electrons.

So, if electron is coming here and when it is transmitting at the same energy level, if there is a state here because which can accommodate this electron then only tunneling will take place. So that is why you have this kind of characteristic for current versus voltage. Because voltage lead to the band bending and then you know this basically the state is basically moving accordingly.

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So, in this lecture we have discussed the quantum transport through a potential step and a potential barrier. And we have also discussed how it applies to different devices and to the WKB approximation. Thank you very much.