Semiconductor Device Modelling and Simulation
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Lecture – 58
Transfer Matrix Approach

Hello, welcome to lecture number 58. Today, we will discuss of the Transfer Matrix Approach. We will go through the transfer matrix approach then write a Matlab code and use it to study the transmission through a double barrier as we saw in case of resonant tunneling diode.

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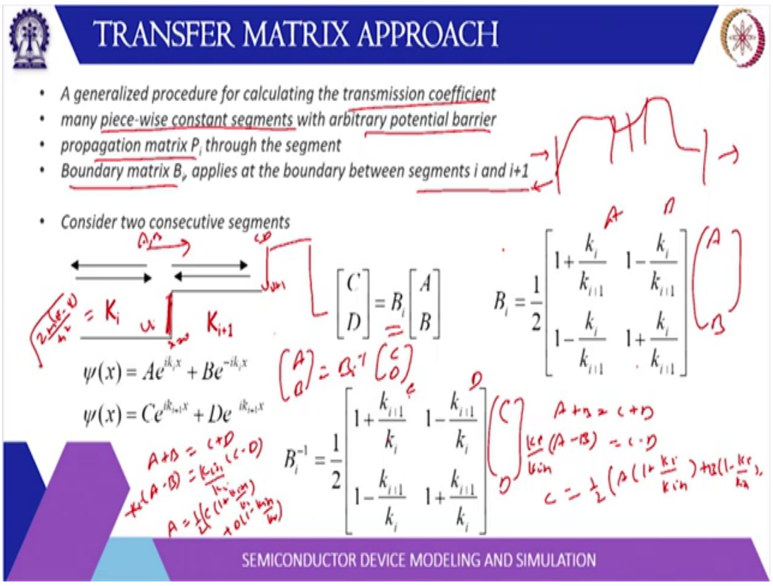

Now, transfer Matrix approach is another way to solve surrounding your equation for multi layered structure. You can assume that for certain segment. The potential is constant and so on. So, the potential is constant for that region of length. L let us say you can define k which is root 2mE – U by h bar square. So, for each segment and let us say U is now U i for each segment. So, here less potentially U i here potential is U i + 1.

Now, these are general procedure for calculating the transmission coefficient and it consists of n number of piece-wise constant segment with arbitrary potential barrier. Now, what we do? There are two things that are defined here, one is for length L of the segment we have propagation matrix P i. And at the boundary of these segments, be a boundary matrix that applies between the boundary elements between segment i and i + 1.

So, let us consider two consecutive segments, so, let us say left section is k i, right section is k i + 1. And on the left section we can write A times e to the power iota kx + B to the power –iota kx. For right side we can assume, let us say, C e to the power iota k i + 1 x + D e to the power –iota k i + 1 x and so on. Now, here we are not using 1 + r and T because this is part of the structure. So, it is not entirely just transmitted wave.

There is another potential here like this, so, there can exist a reflected wave. However, if you consider some potential profile like this, here is only transmitted wave here you will have incident and reflected wave. So, to the extreme right we can assume that there is only a transmitted wave. But in any section in between we have to assume that both the waves exist. So, if you again apply the boundary condition at this region.

Let us say this is basically let us say this is 0 x = 0, so, you can write A + B = C + D and then A – B times k i = k i + 1 times C – D. And then if you rearrange it then you can divide this by k i. So, you can get expression for A, A will be some of these two divided by 2 you will get A so that is C into let us say 1 by 2 C into 1 + k i + 1 by k i + D into 1 – k i + 1 by k i or you can write it like this also A + B = C + D.

And this is A – B into k i by k i + 1 = C – D so, you can get C from here is up at and divided by 2. You will get A times 1 + k i by k i + 1 + B into 1 – k i by k i + 1. So, based on this you can form this matrix that C D = B times A, B. So, this is basically kind of looking forward. So, if you are propagating the wave from left to right so, you can you have A and B you can find C and D at this interface using this matrix Bi.

Similarly, if you are doing other round then you can write A B = B i inverse C D. So that is basically propagating to the left side, basically. So, B i inverse will have 1 + k i + 1 by k i 1 – k i + 1 by k i. So, this basically how it is multiplied. So, this is, let us say, C and D so, this multiplied by C this multiplied by D or here this multiplied by A this multiplied by B. So, this is multiplied by A this is multiplied by B.

As well you can get this is for C. And similarly, you can get for D also, so, this is a simple algebra that you can easily solve and get this matrix. Now, why I am saying this because this is defined for let us say, propagating in x direction.

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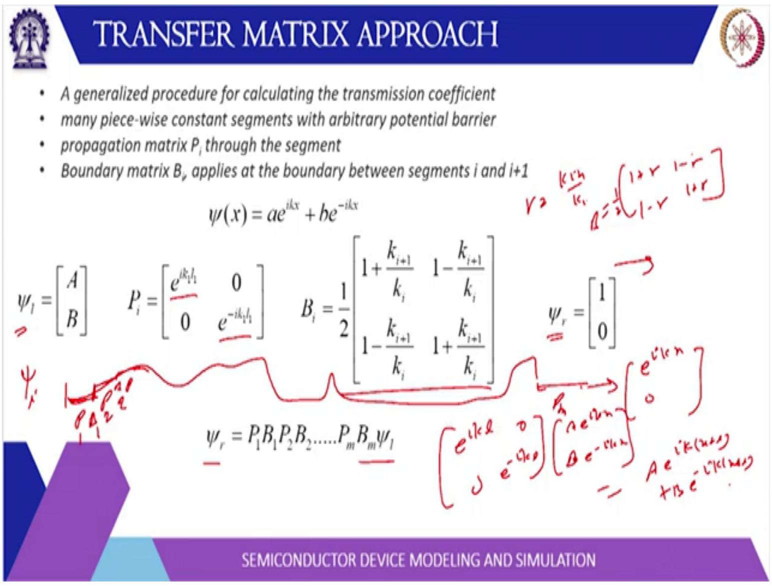

So, let us look at the full picture so on the left side is your psi l which is, let us say A B. And then after this potential profile some profile and right side you have only transmitted wave. So, there is only e to the power iota kx and this is 0 basically. So, only forward going only transmitted wave there is no wave coming from this side. So, this can tell you so, from psi r you can calculate psi l.

How, if you move in backward direction or from psi l you can calculate psi r if you move in forward direction. So, forward direction how will move? For a given section you will apply propagation matrix then there is a boundary matrix then propagation matrix then boundary matrix then propagation matrix and so on. So, psi r is equal to let us say P 1 B 1, P 2 B 2 and so on. And let us say this m section, so, this is P m B m like this times psi l.

Where boundary matrix we have already discussed in the previous slide which is half of 1 + ratio of k of this consecutive segments 1. So, let us say this is r, r = k i + 1 by k i so, this is 1 + r, 1 – r, 1 – r, 1 + r half so, this is your B. And propagation matrix is basically simply the phase difference between the forward propagating and the backward propagating waves. So, if you multiply the let us say some A and B this is e to the power iota k l e to the power –iota k l 00.

And if you multiply just e to the power iota kx B times e to the power –iota kx. So, if you multiply what you get? It is A times e to the power iota kx + l and this is 0 then B + B e to the power –iota kx + l so, simply phase difference of k l is added basically that is it. So, this is the generalized transfer matrix approach.

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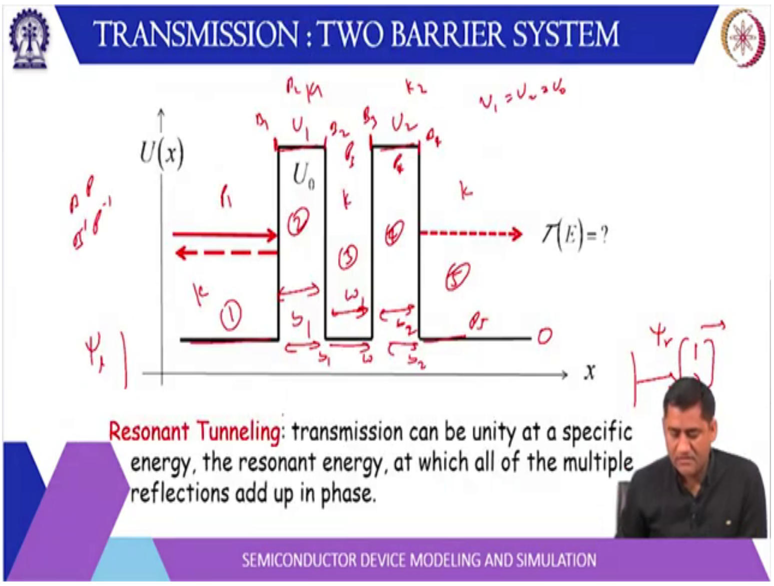

Now, you can apply it to a any problem let us consider a problem of two barriers. So, there are two barriers let us say this height is U 1, this height is U 2. Now, they can be equal it is also possible that U 1 = U 2 = U naught. And then there is a width of this barrier, so, this is a barrier 1. This is well and this is barrier 2 so, width of barrier, barrier 1 barrier 2 and this is the width of the well between the two barriers.

So, how many sections we will have? We can have let us say this is 1 section, this is 2 section, this is 3 section, this is 4 section and let us say this is fifth section. So, here it will be k here will be let us say k 1 here also will be k here will be k 2 and here also it will be k because the potential is 0 here or whatever is the reference value. Then it is length you can assume certain length here.

Let us say this length is B 1, this length is B 2 and this length is let us say w. So, you can have P 1 here then at interface B 1 here then P 2 for this region then B 2 here then P 3 here B 3 here then P 4 here and then B 4 here and then P 5 here. So, what I have done here? To understand the respect I have written one simple Matlab code. But I have made little change. On our right side I am assuming 1, 0 only the transmitted way.

So, only forward propagate wave is there so, from psi r I am calculating psi l. So, instead of B and P, I am taking B inverse and P inverse. If you look here, it is P and B from left to right. So, from right to left it will inverse of this B and P. So that is what I have done. And the sequence will also be different.

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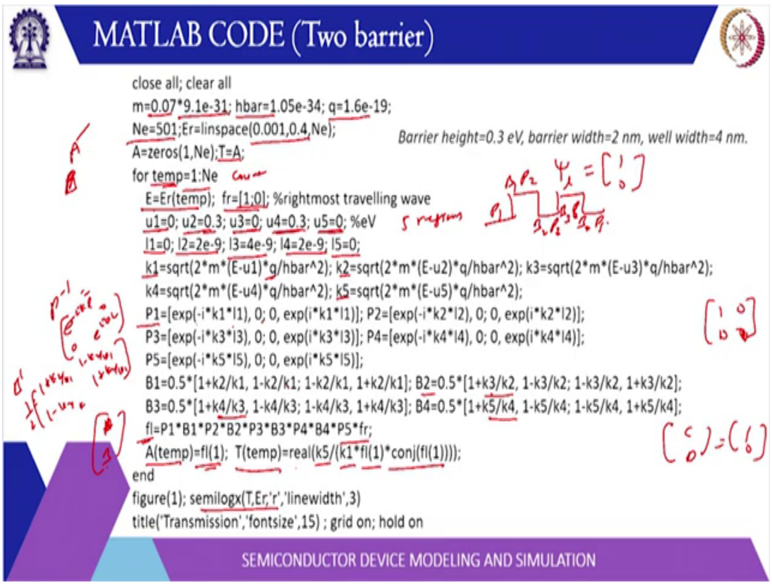

So, mass is taken as 9.1 into e to the power 31 times effective mass. So, at let us say it is 0.07 ideas that if mass is less then this energy will be more spaced basically. So, either you can take less energy or you can change the spacing. So, idea was that you are assuming certain effective mass, whereas there is low mass. And these energies are fairly spaced then h bar then q then energy is taken from 0 to 0.4.

Exactly 0 is not taken means when e is exactly 0 that is not taken for this region because it gives some kind of error divide by 0 but that does not really matter. So, you can start with some arbitrary result small value which is not 0 then number of points is 501. So then we have defined values for A and B so because we are not calculating the reflection coefficient. So, I have only calculated A here.

And along with A I have also calculated the transmission coefficient for each of this energy from 0 to 0.4 electron volt. Now, let us say temp is a count is basically a count for count equal to 1 to any first I calculate take one energy at a time. So, let us say E is the first element of this energy. Then fr is the rightmost traveling wave which I this is basically psi l and which is taken as 1, 0.

So, there is only transmitted wave there is no wave coming from the right side. Then these are the five regions u1, u2, u3, u4, u5. So, here potential is 0 potential is point 3 electron volt a second well is another barrier is another as a right side basically. The length you can take 0 or whatever it does not really matter because it will only cause a phase change. So, it will not cause a change in the transmission coefficient as such.

So, you can take it 0 also, so, this right side and left side this regions length is considered 0 here. Then the well the barrier height is considered 2 nanometre well width is consider 4 nanometre here and again this barrier width also 2 nanometre. And by changing this value we can change the barrier height and the barrier width and the well width. Then for each of the five regions so, there are five regions here.

I have calculated k1, k2, k3, k4, k5 that is root 2mE – U by h bar square and this multiplied by q because it is an electron volt. Then after calculating the k, I am calculating the propagation matrix. Now, this P is basically the inverse of P. So, if you take the inverse of P is a diagonal element, so, each of the element will basically get inverted. So, it is e to the power –iota k l 0.

So, it is basically e to the power –iota k l 0, 0 e to the power iota k L so, this is P inverse basically. So, all five I have calculated so, if you see for region one and five because length is 0, so, this will be 1. So, it is simply identity matrix for reason 5 and this, this is 1, 0, 0 sorry 1, 0. So, this is the identity matrix, so, it will not really change anything for the propagation matrix for first region, fifth region will not change anything.

Then there is a boundary matrix boundary matrix has to be where the reason 1, 2, 3, 4, fifth after that there is no boundary, so, we have only four boundary elements. So, this is 1 + k2 by k1, 1 – k2 by k1, k1 – k2. So, this is basically again this is the inverse. So, B is basically half 1 + k2 by k1, 1 – k2 by k1, 1 – k2 by k1 and 1 + k2 by k1. So, at the interface between 1 and 2 similarly, interface 2 and 3, 3 and 4 and 4 and 5.

Then I can take calculate this the wave function on the left side, so that will be P1. So, it is basically like this P1 B1, P2 B2, P3 B3, P4 B4 and P5 so that is 1 here times fr you get fl. So, f l is let us say you can say this is A and B and they say this is C and D which is equal to 1, 0. So, only transmitted wave is here because this is taken as 1, 0. So now, what I have done here? Because this will have two element one incident one reflected.

So, only the incident one is taken, so, f1 first element is taken which is A and from this I have calculate the transmission coefficient. So that is basically real of k5 by k1 times f1 and conjugate of f1 or I could return A also here. So, A and T both are basically stored. So now, again count = 4 second energy, so, this T matrix is basically a transmission coefficient for all these energies. Then I plotted it on a semilog axis T versus Er.

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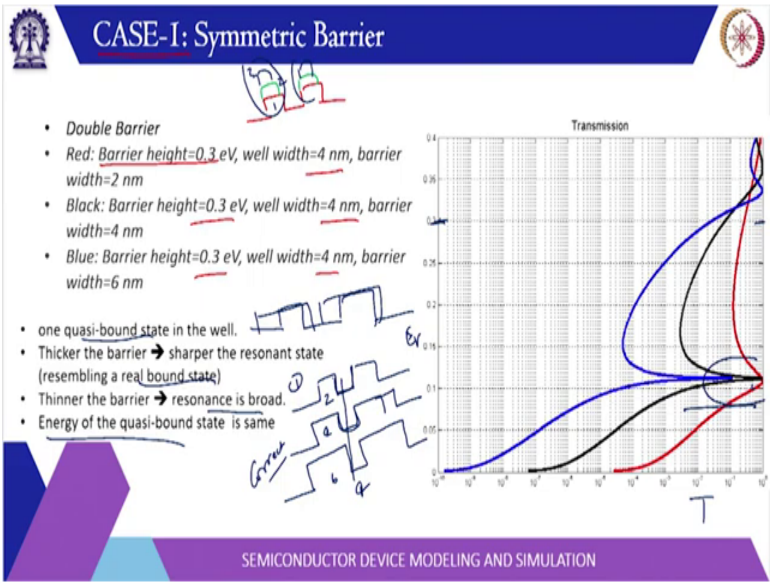

So, here you can see the case that case of that I have studied using this transform matrix approach. So, there are symmetric barriers, so, there are two various of same height, 0.3 electron volt, 0.3 electron volt and the well width is also same 4 nanometre, 4 nanometre only thing that is changing the height of these barriers. So, in first case the height is 2 nanometre in second case the height is let me use different colour second case height is 4 nanometre.

And the third case height is 6 nanometre. So, this is case 1, case 2 and case 3. Now, if you notice here what happens? In case 1 which is red here you see a broad resonance basically. And as the barrier height increases, the resonance becomes narrow, basically. And there is no change in the transmission energy as such. So that means there is a one quasi bound state in the well corresponding to which there is a transmission.

Then as the barrier becomes thick so, instead of this is I have represented as height. So, there is no change in the height I think let me correct it so, this is first case. Then second case is like this, so, height is same and the well so let me write it like this, this is first case. And the second case will be this is a second case and third case is like this. So, this width is always 4 and this is 2, 4, 6 like this height is same.

So, this is the correct one. So, you see as this becomes wide it is basically resembling the real bound state. So, the reason is becomes more sharp. And for thin barrier the resonance is broad and because the well width is same and the energy or the barrier height is same. So, the energy of the quasi bound state remains more or less same. So that is how you get this transmission characteristic.

So, this is basically your transmission coefficient and this accesses the energy. So, from 0 to 4 and the height of the barrier is 3 so, up to 3 this is bounded. So, up to 3 there is only 1 bound sate here the second state is basically above this barrier height, so, this is not boundary state basically.

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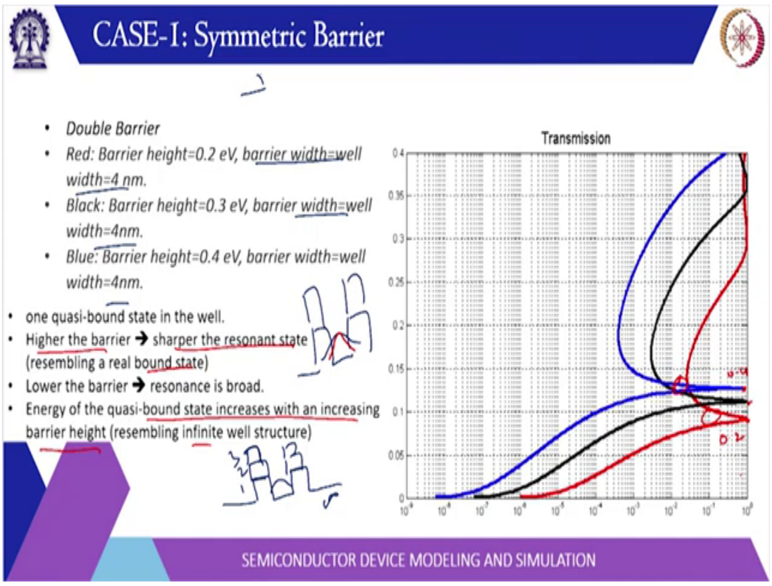

Then in a certain barrier we can also study, the effect of change in the barrier height, so, the barrier width and the well width are same. So, both are 4 nanometre here but the height is changing. So now, this scenario is basically like this. You have let me put it here, so, this is the first case, this is the second case and this is the third case. So, this is what happening here 1, 2, 3.

So, in this case because this barrier height is increasing, so, as the barrier increasing, it is resembling to a infinite potential value. So, in infinite potential value what happens? This energy state is basically more bound so, for high small or barrier height so, let us say this is your barrier. So, this wave function will penetrate here. If you increase the barrier height then this penetration will be reduced.

So, this penetration will be basically reduced now. So, it is more confined, so, it is energy will be actually more. So, we see here for 0.2 electron volt, this energy 0.4, this is 3 reasons 0.4 this is energy, so, 0.4. So, when this barrier height is more, the confinement is more and corresponding bound state energy is more basically. So, there is one quasi bound state and for higher barrier resonances sharper.

And it is resembling the bound state and energy of the quasi boundary state increases with increase in barrier height. So, it is resembling infinite quantum value. Another thing you can notice here, this resonance is sharp see it was broad here it is sharp here. So, it is basically because it is remembers the real bound state. So, for symmetric barrier we obviously two cases one where we vary the width of the barrier second case, where we vary the height of the barrier.

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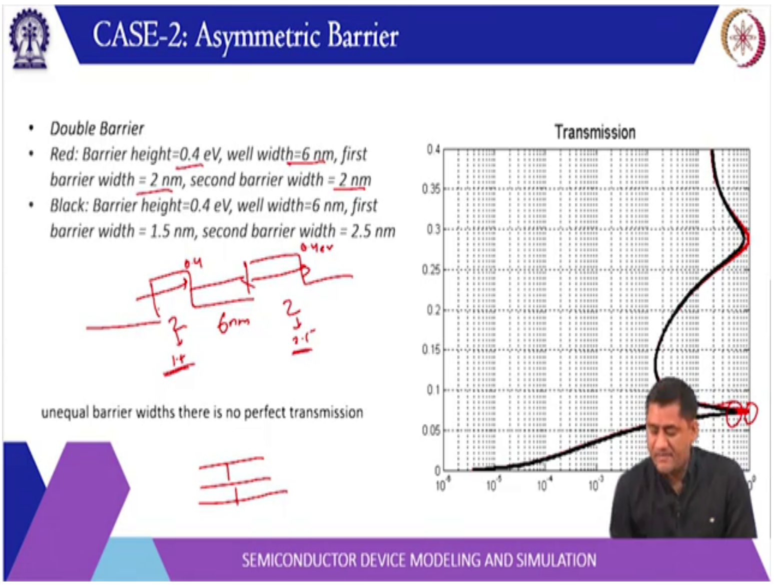

Now, let us consider the asymmetric barrier, so, here there are two cases, basically. In the first case, barrier height is 0.4 well width is 6 and the first barrier width is 2 nanometre second barrier with this also 2 nanometre. So, this is the situation like this, you have barrier height is same. So, this is 2, this is 2 and this is 6 nanometre and height is 0.4. Now, what is done here?

Height is remains same well width remain same this is made 1.5 and this is made 2.5 secondary. So, the barrier which is basically sends so now, the both the barriers are not symmetric they are asymmetric. And that can happen due to some change in the process because when we are growing the multilayer structures like aluminum, gallium, arsenide, like that. There may be one monolayer difference.

So, in that case you can obtain this kind of asymmetric barrier. Now, in case of asymmetric, where you see here for symmetric barrier almost perfect transmission is there, it is going to one. But as soon as the barrier becomes asymmetric, it is no longer a perfect transmission it is slightly less than 1. Now, why it is happening? Because their characteristic have now changed. So, earlier this was exactly the same place.

Now, from the both barrier side, there is certain change to the synergy level. So, the penetration may be same but the width is different. So, the transmission through this barrier will be less transmission through this first barrier will be more. So, they are kind of two barriers which are close by and they are interacting barriers you can say. So, for asymmetric barrier there is some reduction in the transmission, basically.

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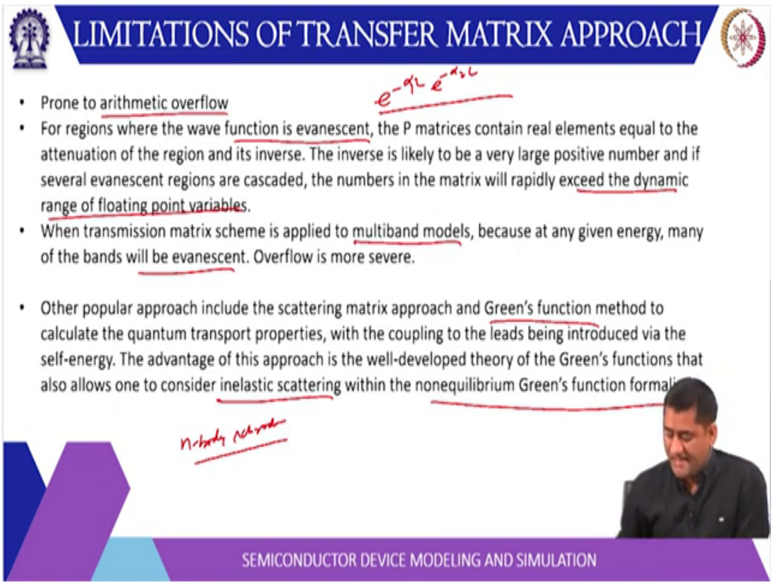

Now, what are the limitations of this transfer matrix approach? It is prone to arithmetic overflow. And what is arithmetic overflow? When number is beyond the description of the computer, basically so because computer represents the number in terms of bytes. And if number is more than that or less than the limit then it will basically we said it, we call it overflow. So, it happens when the wave function is kind of evidence.

And that means, there is some e to the power –alpha L. So, some reduction is there and when this number of these let us say e to the power –alpha L e to the power –alpha 2L they come in sequence then the number becomes very small. And the program may not be able to handle this large numerical change. So, it basically exceed the dynamic range of the floating point variable.

Now, this may happen in the single band model also but for multiband model it is more frequent. Because there will be many bands which will be evanescent. So, overflow is more severe. Now, apart from transfer matrix approach, there are other approaches which take care of this quantum transport. So, once such method is Green's function based method, so which basically calculate the quantum transport property.

And we are coupling that leads to the being introduced by the self energy at the contacts. Then for Green's function approach there is a well developed theory of Green's function that allows one to consider inelastic scattering within the non equilibrium Green's function formalism. Another approach is basically, you can solve n bodies, Schrodinger equation. So that is used for a small number of particles not many particles because that is computationally intensive.

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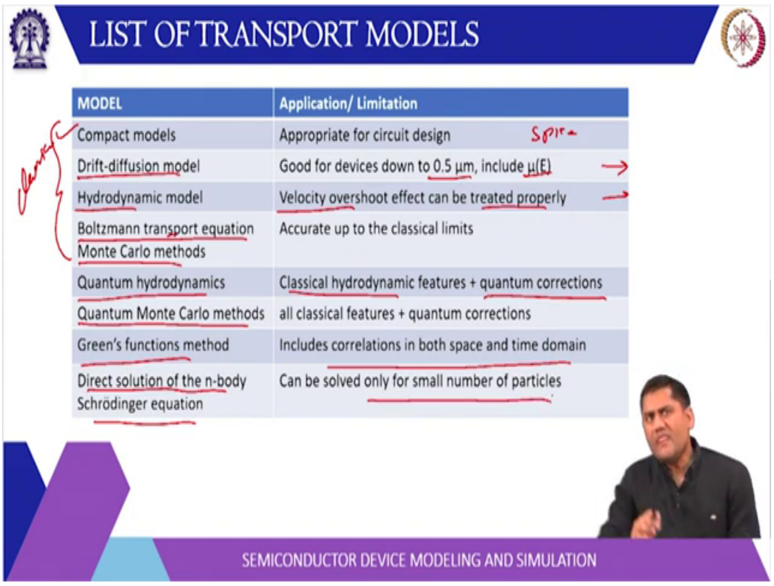

So, I have given you some kind of overview of the quantum transport. But it is possible that you may encounter different models within the same range. So, let us recall all the models that we have discussed. The first is the compact model, so, they are appropriate for the circuit design. So, there they are basically obtained from the measurement or from the simulation then we have the compact models they are usually in is used in spy simulations.

Then we have the basic model called drift-diffusion model that is good for device up to 0.5 micron and it include them electric field dependent mobility. Then there is a hydrodynamic model that can account for secondary effects like velocity overshoot all those effects can be accounted. Then if you want to reach the classical limit then you can directly solve the Boltzmann transport equation and that is done through Monte Carlo method.

So, these are all classical models basically, these are classical models. Now, you can do some quantum correction to these models, so, this will have quantum hydrodynamic or quantum gradient models, they are quantum corrections. So, this is called quantum hydrodynamic model. So, all classical hydrodynamics features plus quantum correction. As discussion in one of our lecture.

Then of course you can do the quantum correction to Boltzmann transport equation, so that is called quantum Monte Carlo method. Then of course, Green's function method it includes a correlation in both space and time. Then of course, finally, the direct solution to the Schrodinger equation it can be solved only for a small number of particles. So, these are the brief summary of the models.

So, what we will do? In next week, we will take up some examples from the commercial simulator **(()) (26:57)** and maybe couple of devices that we can simulate where we can compare and use these models. So that is what we will do in the next class.

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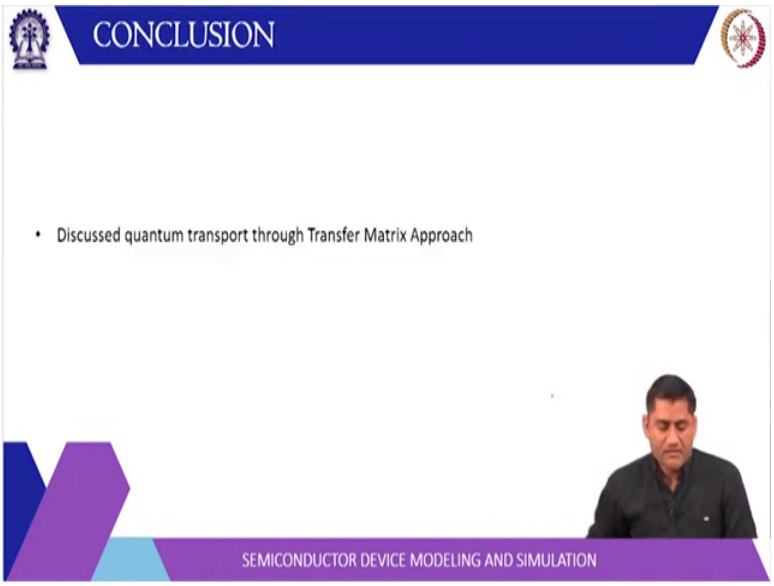

So, in this lecture we have discussed the quantum transport through transfer matrix approach and we have summarized different models. So, whatever we have discussed today, up to today that basically covers the theory. Now, in next week, we will consider some examples how to use them. Thank you very much.