# **Introduction to Semiconductor Devices Dr Naresh Kumar Emani Department of Electrical Engineering Indian Institute of Technology – Hyderabad**

# **Lecture - 03 Electrons in Infinite and Finite 1D Potential Well**

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Schrodinger equation is simply a second order partial differential equation. So, why is it second order? Because, this is the equation shown here. So, what it has is a second order derivative, so, second derivative second order and then there is, you know its partial derivative partial differential equation because we are only showing right now in terms of x.

You could also have dependence on y and z but right now, we are just showing you from the partial derivative with respect to x. So, second order partial differential equation. What is it telling us? Basically, it has some derivatives, and you know this you might have recognized this quantity ψ which is what we called as wave function but this essentially tells you how the particle moves.

We said Schrodinger equation is essentially the analogue of Newton's second law. So, where you know the  $\psi(x)$  describes a particle. It is a wave function of a particle and  $V(x)$  is basically the potential energy of the system. So, basically it is how the potential is changing in a system. So, that is  $V(x)$ , I should call it potential energy simply the potential of the system and then when I know the wave function, I can actually find out what is the probability of finding an electron by calculating what is ψ.

You know if you have ψ, you take the modulus of it and square it that is the probability of finding a particle at a position x. This is finally what is physically observable. Physically, we cannot find, you know wave function. We will only find the probability of finding an electron or a proton or whatever. Correct. And E is the various allowed energy levels in the system. So, with these parameters, you could write an equation of this form and this essentially is what is called as Eigen value problem.

You will study it if you have already not studied it but for now, you just accept this. You know this is a very important class of problems which are called as Eigen value problems. Where whenever you study matrix theory, you will study this. So, what happening here is you have certain you know differential terms and you apply that on the wave function  $\psi$  and when you do that what you get is the wave function again, you get back the wave function.

And then the coefficient is basically what is called as energy Eigen value. So, it is energy of the system. So, this form of Schrodinger equation is called as time independent Schrodinger equation. There is another form which is called as time dependent Schrodinger equation but that is not really necessary for us. So, I did not even mention it. We will not worry about that in this course.

So, this is the time independent Schrodinger equation and we would like to solve this to understand how different, you know material properties change and in today's lecture, we will try to solve this in 2 cases.

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The first case is what is called as the free electron problem. So, let us assume that you have a free electron by which we mean that there is no potential applied anywhere. So,  $V(x)$  is taken to be 0 now. If you take  $V(x)=0$ , you can solve this and find out what is  $\psi$ . That is essentially what is called as for solving the Schrodinger equation. So, how will we do that. So, once  $V(x)$ goes to 0, we can rewrite this V.

It will turn out to be,  $-\frac{\hbar^2}{2m}$  $2m$  $\partial^2$  $\frac{\partial^2}{\partial x^2} = E \psi(x)$ . This is the equation. We can rearrange it a little bit and this can be written as. I will just take the  $2m$  $\frac{2m}{\hbar^2}$  other side so, basically  $\frac{\partial^2 \psi}{\partial x^2}$  $\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2}$  $\frac{mE}{\hbar^2}\psi=0$ . So, this is the equation that we need to solve. Before we solve that we will introduce a constant.

Let us say, we will call it k.  $k^2 = \frac{2mE}{\hbar^2}$  $\frac{mE}{\hbar^2}$ . k will be root of it. We will come to, you know, why this is like this. So, now if I do this, so, basically my Schrodinger equation becomes

$$
\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi(x) = 0
$$

So, what is the solution for this? What is  $\psi$ ? k is a constant. So, what is  $\psi$ ? To find out what is ψ, you know, we have to make some you know guess.

Let us say, let us assume that you know  $\psi(x) = e^{ikx}$ . Let us try to substitute and see what happens. Does this ψ satisfy the Schrodinger equation? How do we do that? So, you take the second derivative essentially you get  $(ik)^2 \psi + k^2 \psi(x) = 0$ . So, basically this particular solution is satisfying the Schrodinger equation.

Similarly, you could also check you know that  $e^{-ikx}$  will also be a solution to the Schrodinger equation. So, both these are solutions to Schrodinger equation. But, what is  $e^{ikx}$  or  $e^{-ikx}$ ? So, these are what we call as plane waves. You know,  $e^{ikx}$  essentially tells you a plane wave which is propagating in the positive x direction whenever there is a wave propagation its  $e^{ikx}$  in this case.

So, basically the general solution would be  $\psi(x)$  because we have 2 solutions which are acceptable. So, we can write a general solution by taking the linear combination of these solutions. So, we can write  $\psi(x) = Ae^{ikx} + Be^{-ikx}$ . So, this is the general solution of Schrodinger equation. So, I mean we could also try to write it in a slightly different form because we know from trigonometry that  $e^{ikx} = \cos(kx) + \sin(kx)$ .

And similarly  $e^{-ikx}$  also, we know what it is. So, you could write it in another form, you know I will try to change the coefficients, redefine the coefficients. I say  $\psi(x) = C\sin(kx) + D\cos(kx)$ . So, this is also a solution. I mean basically these are again some coefficients, some constants. I can define them, you know in terms of A and B and all that we can just compute that.

So, basically these are 2 forms of solutions which are satisfying the Schrodinger equation for a free electron. So, it turns out that the second form is actually much more very suitable for us. So, we will just like you to note this equation now. So, this is the first problem for Schrodinger equation. It is not that complicated. It sounds heavy but it is not that complicated right. **(Refer Slide Time: 08:00)**



So now, what we will do is we will try to understand what it means. So, we redefined you know, we defined k as basically,  $k^2 = \frac{2mE}{k^2}$  $mE$ . So, the reason we did that was; if you rearrange it,  $\hbar^2$ you could also write energy as,  $E = \frac{\hbar^2 k^2}{2m}$  $2m$ . So, what it means is, we know classically, you know in the classical mechanics, we know that kinetic energy is basically,  $K_E = \frac{1}{3}$  $\frac{1}{2} mV^2$  that you could also write it as,  $K.E = \frac{1}{2}$  $rac{1}{2}mV^2 = \frac{P^2}{2m}$  $2m$ .

We studied this in classical mechanics. So, essentially energy in quantum mechanics can be written as  $E = \frac{\hbar^2 k^2}{2m}$  $2m$ . So, this is known as the dispersion relation for a free electron.This is important. Now, what is this telling us? Essentially, you could study this by plotting E versus k. Now, where I will say E is basically energy versus k, k basically captures how the momentum is changing.

So, this is essentially momentum which is  $\hbar$ k. So, how is energy changing with momentum that is captured by this E-k relation or energy momentum relation and it turns out to be a parabola. So, what this is telling you is that if you have a, you know positive k, it is essentially capturing how the energy is you know changing for a wave which is propagating in the plus x direction  $e^{ikx}$ .

So, what this is telling you is that as you change k, the energy is continuously changing. So, for every small change, there will be a continuous change in energy. This is an important characteristic. Similarly for the negative k, we are essentially talking about a wave which is

propagating in the negative x direction and it also has energy which is changing continuously and since  $k^2$  is there, it is basically a mirror image. So, this is a dispersion relation for a free electron.

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It turns out that if you could confine this electron instead of making it free, if you confine it, it has some very interesting effects that is what we would like to do now. So now, we would like to solve what is called as particle in an infinite 1D potential well only because we are only talking about x direction. So, what we are trying to solve is we are saying that an electron is confined to a region of space in x direction, let us say, it is confined to a length L.

So, this is the length L. This is the distance L. So, I will say that electron has to be confined to this region; we are calling it region II here. It has to be confined. It cannot go into either region I or region III which are essentially potential barrier. So, this is a barrier and this is also a barrier region that means electron cannot go there. You can think of it like you know, there is a potential which is basically repelling the electron to stay in the well region.

And this potential is assumed to be infinity in the region I and III that is why you know we are showing that it is a infinite potential and then in between that there is a small well which is of the length L. So now, we would like to solve this. This is equivalent to telling that let us say you know if I have to give a physical example, let us say, I have this you know, pen. I would like to solve how, you know if an electron is confined to this pen itself.

It cannot go anywhere else. So, essentially I am talking about barriers which are surrounding the pen and then electron is only confined to the central region. It is a similar problem here. So now, before we solve this, let us try to ask a simple question which is what is a wave function in the regions I and III. So,  $\psi(x)$ , we said that basically wave function is essentially a function that tells you that you know like you know it can be a  $sin(x)$ .

Essentially, it is a function of x. So, what is it in the regions  $x\le 0$ . Region I means  $x\le 0$  and region III means  $x>L$ , what is a wave function? We are clearly telling you that the wave function and the electron cannot exist in those regions. So, that means there is no probability of finding an electron in that. So, wave function has to be 0 in those regions in I and III.

Why? Because if wave function is non-zero, then the probability which is given by  $|\psi|^2$  is also non-zero that means electron can exist in that region which is not allowed by the definition of the problem. We have taken infinite potential barrier. So, it cannot exist. So, that is why you know this wave function turns out to be 0 in these regions, region I and region III.

Now, part of the problem is solved. Now, if you find out what is a wave function in region II. The problem is fully solved.

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So, what is the wave function in the region II? How do we solve that? Well, in region II, the potential  $V(x)=0$  here. So, the way it is given. This is basically potentially 0 here and infinity on the other side. So, basically  $V(x)=0$  in region II. So, only in region II, you could say that this is  $V(x)=0$ . So, we know what the solution is when  $V(x)=0$ . We have already done this for a free electron.

So, we know that  $\psi(x) = C\sin(kx) + D\cos(kx)$ . So now, what are the coefficients C and D? If we know those coefficients, we are done. The problem is fully solved. To understand that we need to apply what are called as boundary conditions. So, we need to apply boundary conditions by which we mean that we know that you know,  $\psi(x=0)$  is how much.

So, well, we said that  $\psi(x\leq 0)=0$  and the wave function has to be continuous that is one of the properties you know requirements of wave function. So, it has to be continuous. So, at  $x=0$ ,  $\psi(x=0)=0$ . Similarly,  $\psi(x=L)=0$  because again, the wave function  $\psi$  is a continuous function. We cannot have sudden changes in  $\psi$  that is not allowed by the equation.

So, basically since I has to be continuous, these 2 boundaries at this 0,  $x=0$ ,  $x=L$  wave function has to be 0. So, will that help us solve the problem? Well, it does because if you have cos dependence in the wave function, then at  $x=0$ , it cannot go to 0 at all, if there is a cos because cos.  $Cos(0) = 1$  so it always will be non-zero at  $x=0$ .

So, if your wave function you know, the equation 1 because of this, sorry not, boundary condition 1 because of this implies D=0 because if D $\neq$ 0,  $\psi$  will basically be non-zero that is why D=0. So, now the wave function simplifies to  $\psi(x) = C\sin(kx)$ . Now, we have the second condition which is at x=L, so basically  $\psi(x = L) = C\sin(kL) = 0$ . This has to hold for any k.

So, what kind of relation should it be? So, basically this implies that  $kL = n\pi$  only when the variable in the sin function is equal to  $n\pi$ . We can be assured that the sin function goes to 0 at any k. So, this implies that  $k = \frac{n\pi}{l}$ L . This is an important relation. So, what we are seeing is k, the free electron k, k was continuous function you could take any value of k and then there will be corresponding energy.

But the moment you confine an electron to a small potential like this, k cannot be a continuous function. k has to be discrete because L is fixed and  $\pi$  is a constant, n is an integer. So, it can only take discrete values. So, we write it as  $k_n = \frac{n\pi}{l}$ L . Just to make sure, just to denote is the same k but when we write  $k_n$  we are trying to say that there is a discrete  $n = 1, 2, 3, \ldots$ .

So, this is the discreteness that has come about in k. This is an important consequence of the confinement of an electron.





So, if you confine, so what does it mean? Now, I have simply dropped C because C is basically what is called as normalization constant. We can actually find out what exactly it is it turns out to be root 2 by  $\pi$  in this case but like for now, let us not worry about that constant, let us assume that you know this is not truly correct but the functional form of  $\psi(x) = \sin(kx)$ . So,  $k = \frac{n\pi}{l}$ L .

So, I can write my wave function as this for  $n = 1, 2, 3$  and so on. So, what does it mean? We can try to substitute. It we can plot it in Python or MATLAB, just try to do that you will see that the behaviour of wave function  $\psi$  is basically like this. You know, you have at the n=1, you have this half wavelength. At n=2 you have full wave and as n keeps increasing, you have more and more oscillations in your wave function.

And we said energy  $E = \frac{\hbar^2 k^2}{2m}$  $2m$ . Now,  $k = \frac{n\pi}{l}$ L So, energy becomes,  $E = \frac{\hbar^2 k^2}{2m}$  $\frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}$  $2m$  $n^2\pi^2$  $L^2$ . This is an important consequence. Basically now, what we are saying is; the energy is again discrete now. It is not continuous value that is what is shown here.

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So, I have tried to combine the dispersion of a confined electron and a free electron. Please do not get confused. So, this part is basically the negative axis, I am just showing the free electron and on the positive axis, I am showing the confined electron, just to make the difference apparent. So, in the case of a free electron, you have continuous variation. The dispersion is continuous. This was basically  $E = \frac{\hbar^2 k^2}{2m}$  $2m$ .

Whereas if you confine an electron in a potential well of length L, then the energies are no longer continuous. Just the red curve is only for your reference but it turns out that energies are basically discrete and the discrete energy levels are given,  $E_n = \frac{\hbar^2}{2m}$  $2m$  $n^2\pi^2$  $L^2$ .So, you know a discrete case which are allowed. You have discrete amount of energy.

So, this essentially is, why you could say that you know, you call it quantum mechanics. So, essentially energy was continuous in the first case and then it became quantized. You know there are discrete energies which are allowed that is why you have, we call it quantum mechanics. And I would like you to study what happens when you change L. When you do this calculation, you know, I can, we will just do it in a moment.

But if L is large for example  $L=1$ cm or  $L=1$ mm, the energies are you know very, very close to each other. It does not really matter; you know when you go to macroscopic scale. For example, I want to, let us say, I want to calculate the current which is flowing through my strand of human hair. I want it somehow assuming that it conducts, I want to calculate that. Then, the size is 1 micron. It is reasonably large.

Now, large compared to de Broglie wavelength. You know, if  $L \gg \lambda_B$ , you know that is de Broglie wavelength but if you are trying to talk of current conduction, you have talk of electron de Broglie wavelength, we have to take. So,  $L \gg \lambda_B$ , then no need of quantum description. If  $L \sim \lambda_B$ , then quantum description is essential, QM essential, the quantum mechanics is essential.

So, how does L impact? Well. If you confine the electron into a smaller and smaller dimension, then energy goes higher and higher. The discretization becomes stronger and stronger. You could try to put in some numbers and check this for yourself. So, L is in the denominator,  $L^2$ right. So, as L goes smaller and smaller, E becomes, you know larger for same n of course.

So, this could also be understood by the uncertainty principle. We know from Heisenberg's uncertainty principle.  $\Delta x \Delta p \geq \frac{\hbar}{2}$ 2 . So, if you try to confine an electron in a very, very small dimension, its momentum becomes very large. Once its momentum becomes large, the energy also increases that is uncertainty. If your x is large for example  $x=1$ km, then the uncertainty momentum is nothing.

So, energy is very accurately known. This  $\Delta p$  basically tells you what is the uncertainty in the momentum in p. So, if your uncertainty in x is very small that means I know accurately electron is confined to 1 nano-meter space, if I know that, then uncertainty momentum is large. If I know, I do not know, I mean, x is very large, you know uncertainty in x is large for example 1 centimetre, then  $\Delta p$  is very, very small that is it.

It is nothing very complicated. I am just repeating it because I want to drive this point home. This is all, there is to quantum mechanics. If you understand this, you understand quite a bit of quantum mechanics and honestly, you know you could do a lot of things.

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So, let us try to compute this. You know, what is this? What are the energy levels which are there? So, I mean this is just a homework problem, you could try to do it. So, well you are asked to calculate the first three energy levels of an electron which is confined to an infinite potential well of width L=1nm. So, well I mean the formula is known to you. It is just plug and check.

So, you know that energy is basically, just remember you know you do not have to remember these formulas, you know,  $E_n = \frac{\hbar^2 k^2}{2m}$  $\frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}$  $2m$  $n^2\pi^2$  $L^2$ . Substitute. If you do that you will get something like ,  $E_n = n^2(-10^{-19}) J$ 

This is what you get energy in terms of joules you get it like this. So, this is not a very convenient thing. So, what we do is we try to do you know compute energy. We try to give energy in electron volts, units of electron volts. So, basically the way we define that is 1 electron volt which is again another unit of energy  $1 \text{eV} = 1.602 \times 10^{-19} \text{J}$ .

We use this. So, please you know make note of this. So, sometimes you know we refer to energies because eV is a very convenient unit for electron bands and all that. So, electron volt, 1 electron volt is basically 1 point, you know charge times charge joule, know, q joules you can say. So, if you do this calculation, you will get this, you know. Please try to do it yourself.  $E_1=? E_2=? E_3=?$ .

So, I mean, I think, this would turn out to be something in the range of, I I am not very sure but it should be something like 0.32, I think 3.5 or something, in that range you will get some numbers. So, please try it out and verify that you are getting this correct orders of magnitude. These are typical numbers. If you reduce  $L=0.5$ , the number energies will increase you can do all this.



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So, this is basically about how electron behaves if it is confined to a potential well. But in real life, we will almost never have an infinite potential, always the potentials are going to be finite. So, we can also talk of a finite potential well which is very, very close to an infinite potential well. In the infinite potential well, in the earlier case you know in this picture, I have shown you the wave functions which are simply going  $\psi(x) = \sin\left(\frac{n\pi}{l}\right)$  $\frac{m}{L}x$ )

You could also calculate the probability of finding an electron by calculating basically, modulus square of your wave function and if you do that basically what you know the difference for each n basically  $n=1, 2, 3, 4$  and 5, we are showing the wave functions here. So, what this is telling you is that if you confine an electron to a region 0 to L, if the probability of finding an electron is highest at the centre of the; you know it shows this dependence, the probability shows a you know half a independence like this.

It is said to be in the first state energy level 1. If the probability is distributed, for example you know, you have highest probability in 2 locations, this is basically that  $L$ 4 and  $\frac{3L}{2}$ 4 so, at 2 locations you have the maximum probability of finding an electron. It is said to be in the second state and if it is at 3 locations,  $\underline{L}$ 3  $, \underline{2L}$ 3 and  $\frac{3L}{2}$ 3 ; well I mean it should not be that.

You know there is a slight displacement, it is not L right. L is basically is slightly offset but the point is that if you have 3 peaks, it should be third state and 4 peaks, four state and so on. So, this is the probability of finding an electron. It cannot take any other state except this. So, the beauty of it is, the electron we say that the wave functions form a complete set by which we mean that it has to take any of these states or a linear combination of these states but it cannot take any arbitrary function in between.

Anyway, we will have to talk about it later. Now, let us see what happens when the potential becomes finite. It turns out that the problem is very, very similar but to solve this, we have to do a lot more numerical stuff, you know numerical and we can actually do it analytically but it becomes tedious. So, we have used a software. We will try to post it on a tutorial.

We will try to demonstrate this using in one of the tutorials but essentially this is computed using numerical approach in Python. So, what this is telling you is that the wave function of a finite potential will also kind of similar to the infinite case. But the only difference is that you see that in the barrier regions, you know this is again, you know a barrier right. This is a barrier and this also is a barrier. You have barrier regions.

In the barrier regions also, there is a non-zero probability of finding an electron. So, if you look at this, the wave function ψ has a tail in barrier. This is a small probability of finding it and if you go to, you know this probability you know finding you know is called as tunnelling basically. What is it? Actually electron is tunnelling into the barrier regions that is why there is a non-zero probability of finding an electron there.

If you go to the lowest energy states, you see that the probability of finding an electron outside in the barrier is not very significant but as the energy increases for the wave function, the electron increases you see that there is increasingly higher probability. If you compare the area under the curve here, you know this is for the fourth state with the area under the curve.

In the fifth state, you will see that in the fifth, sorry this is the fifth and this is six. This is  $E_5$ right. So, this is fifth state. If you compute the area under the curve here this location and compare with this, you see that there is a higher increasing tunnelling basically or increasing probability of finding an electron outside. So, we will use this to explain because you know I could actually take you know I could say that in semiconductor, there are valence bands and conduction bands.

And I can go on from there but it is not very intuitively satisfying. So, I am trying to build up how energy bands come about in semiconductors. We will do that in the next lectures, next couple of lectures but for now, I would like to stop here today. So, what we did today was? We started out with defining what semiconductors are; what are the basic properties and we said that to understand how this conductivity happens in semiconductors.

It is essential to understand a little bit of quantum mechanics. So, we have done a very, very quick review. Now, we said that quantum mechanics you know you have this probability of finding an electron at some point, you can calculate that and that is given with the wave function and to find out the wave function, you have Schrodinger equation and we took 2 cases.

We took the Schrodinger equation when you know free electron that is potential is 0 and when you have a potential well. We solved that. So, in these 2 cases, we have seen how the wave functions behave and how the energies are changing. So, we said that this idea of quantization or you know discreteness of energies is a very, very important concept. It is central to quantum mechanics.

It cannot occur classically but in a way, it is similar to what you would see; there are some analogue in the classical world also. For example, when you have a guitar let us say. When you strum a guitar, you have a specific note which is produced. Why does a specific note get produced? Because you have a string, you have a string of certain length and then your tight string and then you are plucking it.

So, when you pluck it, it can oscillate only at a certain mode. Depending on the length of the string and the tightness of the string, you could control the note that is you can that you can play on a guitar. So, essentially we are quantizing the sound waves in that case. Of course, we do not need quantum mechanics to explain that we can also because it is large scale, we can explain using classical laws but essentially this idea of you know discrete energies or discrete waves which are allowed is there.

And quantum mechanics also is sort of in a similar direction. So, with that you know I would like to stop here. In the next lecture, we will try to see how you know energy bands form and we will go a little bit more into depth of all these things. So, I hope you understood what you are talking about. If not, please take time to review the lecture one more time and we will meet you in the next lecture. Thank you very much. Have a good day. Bye.