Physics of Nanoscale Devices
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Lecture - 04
Electron in a Potential Well

Hello everyone. In our previous discussions, we have seen that, the electronic devices are shrinking in size and that is basically changing the way electrons behave in these devices. And in order to understand, the new or the nature of electron in our modern devices, we need to understand the quantum mechanical nature of electron and in our previous lecture we started with that discussion.

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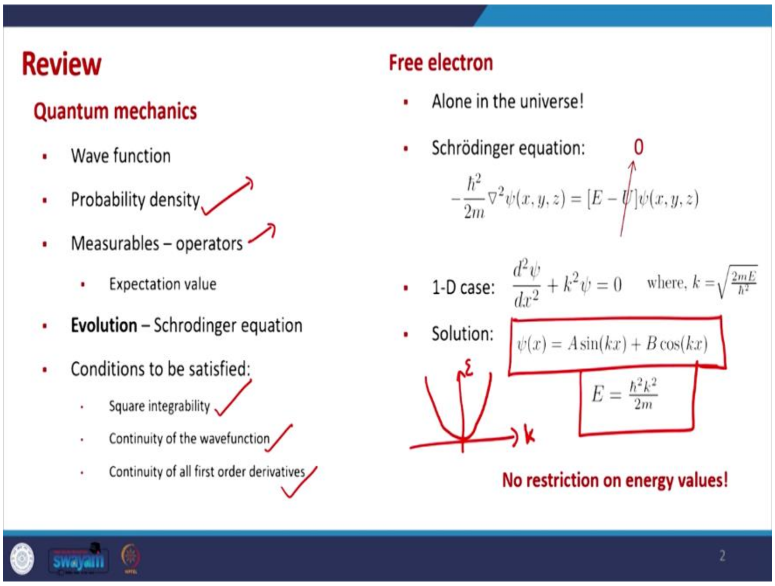

And we started we basically try to understand try to comprehend all the postulates of quantum mechanics. And these postulates of quantum mechanics can briefly be summarized as, that every system has a wave function, but the wave function wave function contains all the information about the system, but it does not directly correspond to a physical entity or it does not correspond to a physical property of the way of the system.

So, the probability density is defined as a way to extract physical information from the wave function. Apart from the probability density, we have other operators known as measurable operators. And these are the operators corresponding to the physical properties of the system. So, for example, for an electron, the operators correspond to the momentum of the electron, the energy of the electron or the position of the electron.

And the expectation value of the these operators tell us about the average value of outcome that we will obtain if we make a large number of measurements on the system. The evolution of a quantum mechanical system is given by the Schrodinger equation. And the wave function needs to satisfy a few conditions.

For example, the square integrability and related condition is normalizability, the wave function should be continuous, it is first order derivative should be continuous. And this we discussed in the last class as well. Apart from the basics of quantum mechanics, we also discussed how a free electron behaves and a free-by-free electron, we mean that the potential energy of the electron is 0.

So, we solve the Schrodinger equation for a free electron and we saw that, that the E-k plot for a free electron is basically a simple parabola. And the wave function for a free electron is a superposition of sine and cosine functions.

And there is this parameter k that comes into picture, this is a function of energy of the electron. So, this is what we saw in the last class. This was a very. So, to say this was a very simplistic description of the electron. No electron in the universe is free. So, now, we will try to see, what happens when the electron is confined in a potential or electron is interacting with other systems.

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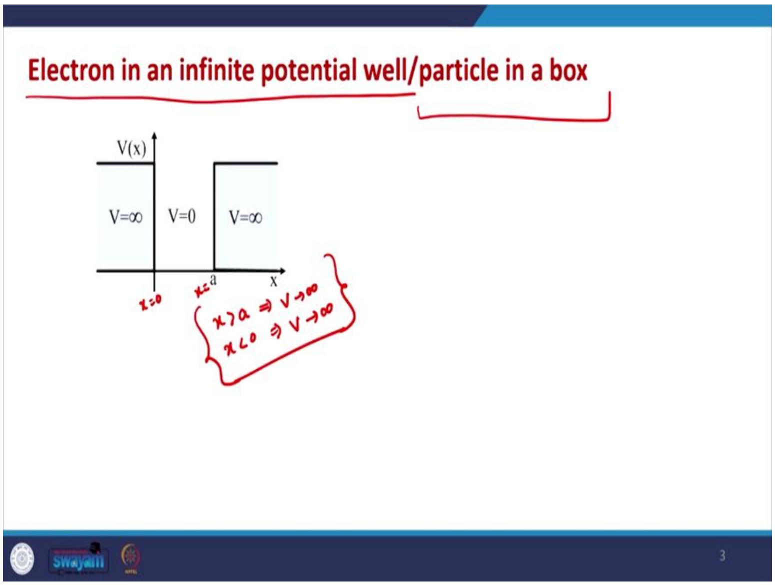

And, in order to understand this concept, we will study electron in an infinite potential well. So, electron in an infinite potential well, problem is also known as the particle in a box problem. So, in this condition, the electron is relatively free in a small region of space.

So, for example, in this case this is 1-D infinite potential well and in this in this potential well, the electron is free in a small region from x equal to 0 to x equal to a. So, in this region, the potential or the potential energy of the electron is 0 and apart from this region, the potential is infinite.

So, for x greater than a, the potential is infinite. And for x less than 0, potential also is infinite. So, this is known as the electron in a potential well or particle in a box. You might be thinking why are we studying specifically this problem. Let me clarify this in the beginning itself, electron is confined in solids. So, electron is tied to an atom, to it is basically the force between the nucleus of an atom and the electron ties the electron and it is like electron is being confined by the nuclear potential.

Secondly, in modern day heterostructures also, the electron is sometimes confined between the interfaces, between a certain boundary of the device. So, this kind of situation happens in modern devices and this kind of situation not exactly this, but similar to this happens in an atom as well, ok. So, that is why we will study, we will start our discussion with a, electron in an infinite potential well.

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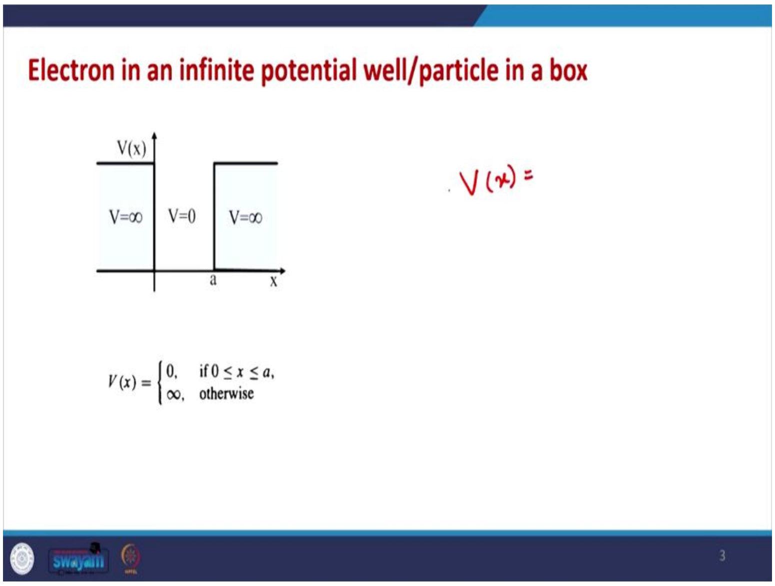

And as all of us can see, the potential energy of the electron in this case, can be written as.

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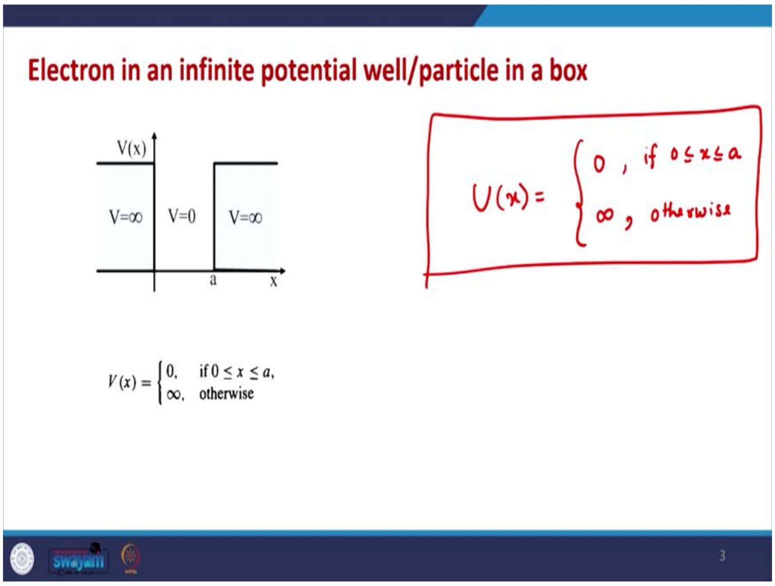

If we write U as the potential energy of the electron, it can be written as 0, in the space between x equal to 0 to x equal to a.

$$U(x) = \begin{cases} 0, & if\ 0 \le x \le a \\ \infty, & otherwise \end{cases}$$

And the potential energy is infinite, in all other regions. So, this is the potential energy of the system. Now, we just need to solve the Schrodinger equation for this system in order to understand the behaviour of electron in this potential well.

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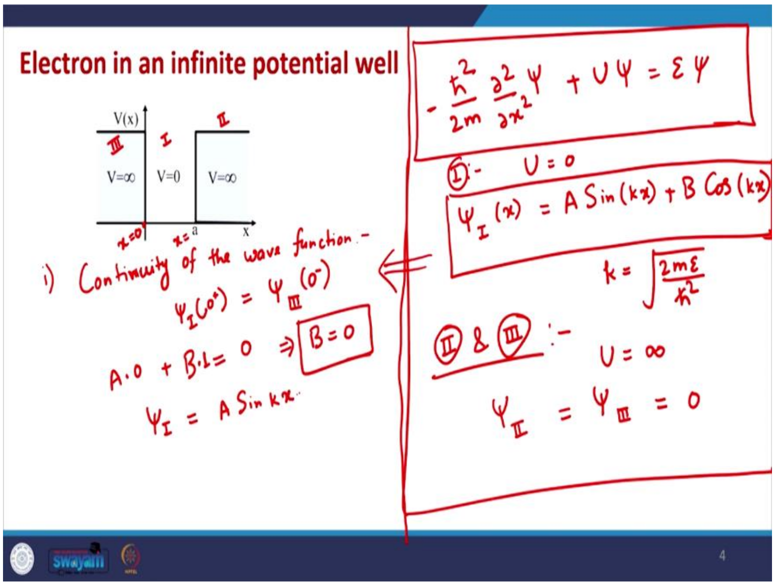

So, we will start with the solution of time independent Schrodinger equation, which basically reads as minus h square by 2 m del 2 by del x square psi plus U psi equals E psi.

$\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \widehat{U}\right)\Psi = i\hbar\frac{\partial}{\partial t}\Psi$ ... So, if the energy of the electron is fixed and it is E, then in this case, we just need to apply the Schrodinger equation to various regimes, ok.

So, if we mark the regimes of the potential well as 1, 2 and 3. In region 1, the potential energy is 0 and the electron is as if it is a free particle, free electron and as you might have already guessed the wave function of the electron in region 1, will be given by Asin(kx), directly from the solution of the free particle equation plus Bcos(kx), ok. In region 1, the electronic wave function will be just like a free particle solution and this we have already derived in our previous class.

So, this parameter k is again the same parameter, the wave number and it is given as square root of 2 m E divided by h bar square $k = \sqrt{\frac{2mE}{\hbar^2}}$. Here A and B are unknowns, which we will eventually find out in this case. But let me pose a question to you here, what will be the electronic wave function in region 1 and region sorry in region 2 and region 3?

What will be the electronic wave function in these 2 regions? Region 2 and region 3. Just take a moment and think about this, as you can clearly see, the potential energy of the electron is infinite in these two regions.

Which basically means that, in order to exist in these regions, the electron needs to have infinite amount of energy. So basically, the electron cannot exist in these regions physically. So, the wave function in region 2 and region 3 will be 0. It means, that the electron cannot exist in these regions physically, ok. So, from the Schrodinger equation and from the common sense I would say, we have, the electronic wave function in various regions of the potential well.

So, now we just need to apply the boundary condition on the wave function of the electron. So, the first condition is the continuity of the wave function. Continuity of the wave function. And as you can see, there are two boundaries in this system one is at x equal to 0 and second is at x equal to a.

So, the wave function in 0 plus $\Psi(0^+)$ should be equal to the wave function at 0 minus $\Psi(0^-)$. So, just before x equal to 0 and just after x equal to 0, the wave function should be equal to each other; in order to satisfy the continuity condition.

And as we can see, from these equations, $\Psi_I(0^+)$ is basically, when we put x equal to 0 in $\Psi_I(x)$ expression, in that case, it would just be this the first term will be 0 and the second term will be. So, it would be A times 0 plus B times 1 equals Ψ_{II} is 0 always. So, this will mean that, B is equal to 0, ok.

So, the wave function in region 1, will just be Asin(kx), ok. Now, we will apply the second boundary condition, to the system and we will see that this also gives us some interesting insights about the system.

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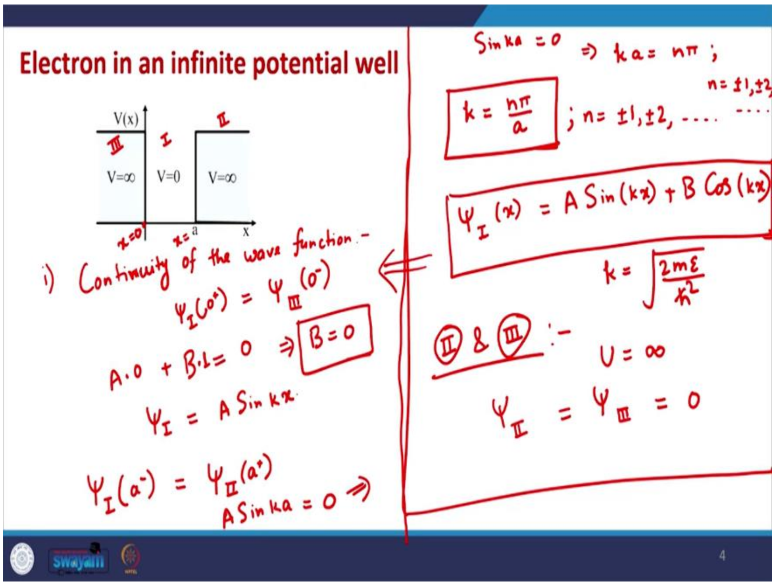

So, applying the boundary condition at x equal to a, the wave function just before x equal to a, which means $\Psi_I(a^-)$ should be, equal to the wave function just adjacent to the x equal to a on the right-side $\Psi_{II}(a^+)$.

This left-hand side now is, Asin(ka) and the right-hand side is 0; because psi_2 is always 0; which means that, sin k a should be 0. It implies that k a should be n pi, where n can be any integer, it can be plus minus 1, plus minus 2 or any integer. So, what it basically means, that k is now n pi by a; where n is n integer number, ok… $k = n\frac{\pi}{a}$ $\quad n \epsilon$ I

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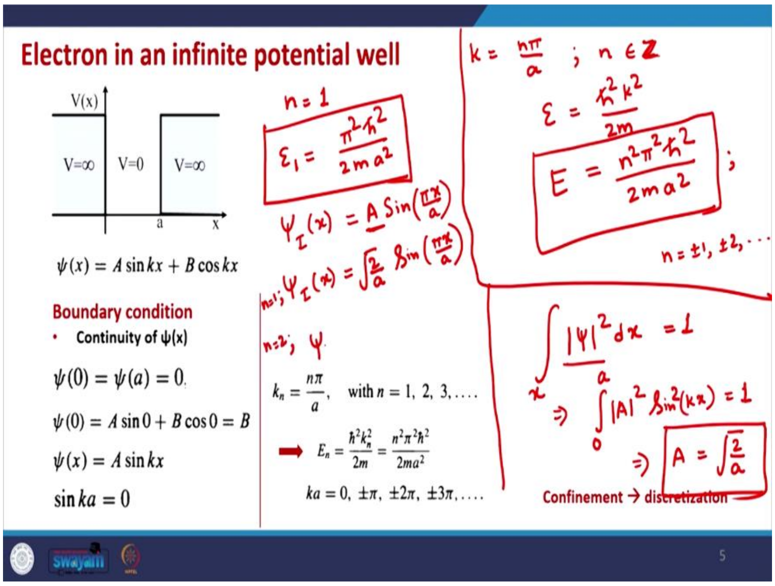

So, to summarize this, in a potential well problem, we have, k equals n pi by a, where belongs to the set of integers, ok. And what it immediately implies is that, the energy of the system which is basically h bar square k square divided by 2 m $\left(E = \frac{\hbar^2 k^2}{2m}\right)$, is now n square pi square h bar square divided by 2 m a square $E = \frac{\hbar^2 \pi^2 n^2}{2ma^2}$, where n is now a discrete thing it is just an integer or if we take a positive value, it is a natural number.

So, what it immediately means is that, the energy now cannot take, all possible values. As the energy of electron could take all possible values in case of a free particle, free electron in this case the electron cannot take all possible energy values. Electronic energy values can only be discrete now. And that is an interesting outcome because, as soon as the electron is confined, it means that the energies of the electrons or energy of a single electron is getting discretized.

So, if we look at if we put n=1 in this case, the energy of the electron would be $E = \frac{\hbar^2 \pi^2}{2ma^2}$. So, this is the first allowed energy value of the electron. And the wave function corresponding to this is, corresponding to n=1 is $\Psi = A\sin(\frac{\pi x}{a})$. So, $\frac{\pi x}{a}$, this parameter a can be determined from the normalizability condition, by normalizability we mean that, the probability of electron being found in the entire space should be 1.

So, the this is the probability density. The integral of probability density over entire space, gives us the probability of electron being found at all places or anywhere and as we know that, in an infinite potential well, the electron cannot be found beyond a and before 0.

So, this integral basically boils down to integral from 0 to $A^2 sin^2$(kx) equals to 1. So, if we solve this integral and this is a small homework exercise for you, please solve this equation. This A value turns out to be $\sqrt{\frac{2}{a}}$, ok. So, this electronic wave function, for n equal to 1 is given as, $\sqrt{\frac{2}{a}}\ \sin(\frac{\pi x}{a})$, ok.

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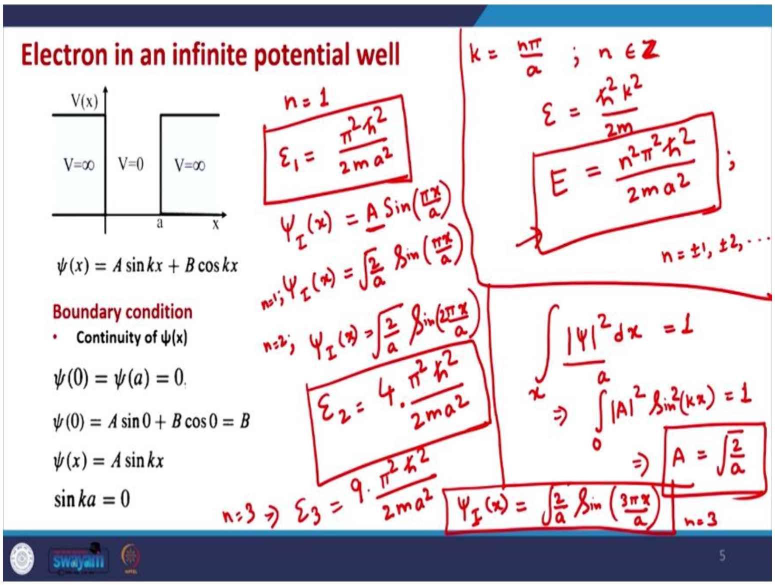

And similarly, this is for n =1, for n =2, the wave function reads as $\sqrt{\frac{2}{a}}\,\sin(\frac{2\pi x}{a})$ just by putting n =2 and energy corresponding to this state will be n square will be in this expression if we put n=2, this would be $E = \frac{4\hbar^2\pi^2}{2ma^2}$.

So as you can see, the energy of the state, is now 4 times the energy of the state when n was 1. And similarly for n =3, the energy of the system would be E_3 would be, $E = \frac{9\hbar^2\pi^2}{2ma^2}$.. And similarly, the wave function would be, $\Psi(x)_{n=3} = \sqrt{\frac{2}{a}}\,\sin(\frac{3\pi x}{a})$. So, this would be for n=3. So, as you have already realized that the electronic nature for when the electron is confined in a potential well is quite different from what it is when the electron is free.

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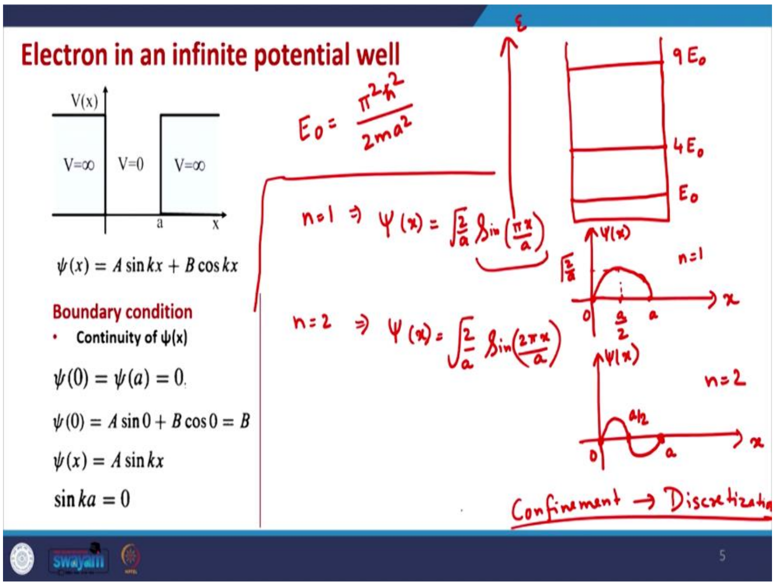

And now, the electron can take only certain energy values. So, for example, if we define E_o to be $\frac{\hbar^2\pi^2}{2ma^2}$, the first allowed state will be having energy E_o. If this is y-axis this is the energy axis, the second allowed state will have energy 4 times E_o and the third allowed electronic state will have energy 9 times E_o, ok. And similarly, 16 times E_o and so on.

So, any confinement; so, in this basic example we have seen that a confinement leads to discretization of energy value. So, what we can say is, that confinement leads to discretization, ok. Apart from this, there is one more interesting observation, that you can have in this system and that is if we put n=1, the wave function of the electron inside the well is $\sqrt{\frac{2}{a}}\,\sin(\frac{\pi x}{a})$.

And if we plot this wave function on x-axis, wave function as a function of x, $\Psi(x)$ versus x, we see that at x equal to 0, this wave function is 0 and again at x equal to a, this is again 0, ok. x=$\frac{a}{2}$ this takes maximum value of $\sqrt{\frac{2}{a}}$. This sin takes maximum value of 1. So, the wave function takes the value of $\sqrt{\frac{2}{a}}$.

Similarly for n=2, the wave function looks like this, $\Psi(x)$ is basically $\sqrt{\frac{2}{a}}\sin(\frac{2\pi x}{a})$.. And if we plot this function, for n=2, $\Psi(x)$ versus x this would be, like this. So, the wave function would be 0 at x equal to 0. The wave function would again be 0 at x equal to a.

But in addition to x=0 and x=a, the wave function would be 0 at x=$\frac{a}{2}$ as well. And if we plot, or sort of if we visualize, these wave functions in the potential well itself.

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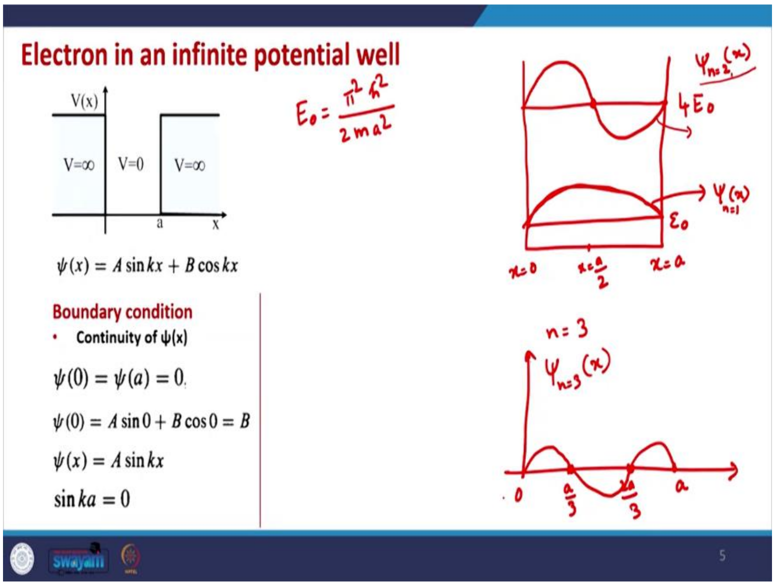

Then what we can see is that, the first allowed wave function looks like this and it has energy E_o. This is the $\Psi(x)$ for n=1. The second allowed, energy is $4E_o$, where E_o as you might recall is $\frac{\hbar^2\pi^2}{2ma^2}$. Now, the wave function looks like this. And an interesting observation here is, that the wave function goes to 0 in the middle of the well.

So, if this is x=0, this is x=a, in the middle of the well, the first excited wave function or $\Psi(x)_{n=2}$ −goes to 0 in the middle of the well. And so, what it means is, that the electron cannot be found in this state at x= $\frac{a}{2}$. So, whenever the electron has energy for E_o or it is having a wave function where n=2 in that case, the electron cannot be found at the middle of the well.

And that is an interesting and counter intuitive outcome which comes from the solution of the Schrodinger equation. And similarly for n=3, if we plot, from x=0 to x=a, in that case, we can see, that electron will have now 2 nodes, 2 points in the well, where it will have a 0 value like this.

So, the if the electron exists in this wave function or electron has energy of 9 E_o and it is in n=3 state, in that case, the electron cannot be found at x= $\frac{a}{3}$ and x= $\frac{2a}{3}$.

So, these are called the nodes in the in the potential well. And these are, these are quite counter intuitive from classical point of view, because if a classical particle exists somewhere, it has energy greater than the potential energy it can exist at that place and it can exist at any such place. But in a potential well problem even if electron has energy greater than 0, it cannot exist in a certain state at a certain point.

So, for example, it cannot exist at x= $\frac{a}{2}$, in this state n=2 state. And similarly, it cannot exist, at x= $\frac{a}{3}$ and x= $\frac{2a}{2}$ for n=3 state. However, it can exist in n=1 state at all these points. It can exist at these points for other values of n as well, ok.

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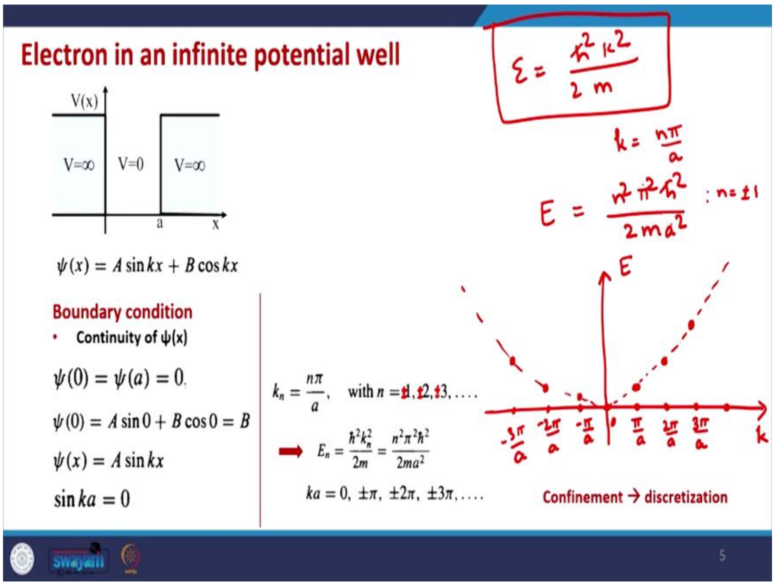

Finally, if we look at the E-k relationship now, which is quite an important relationship in solid state physics. The E-k relationship will be, the E-k relation mathematically is the same, it is still $\frac{\hbar^2 k^2}{2m}$. But now k values take the, discrete the k can only take the discrete values.

So, this, the relationship between E and k can be rewritten as, $\frac{n^2\hbar^2\pi^2}{2ma^2}$; and if we plot, the E k relationship, where this n can be any integer. Actually, it can be any integer, in the slides as well. So, if we have k on the x-axis and E on the y-axis, the electron can only take wave numbers, which are multiple of $\frac{\pi}{a}, \frac{2\pi}{a}, \frac{3\pi}{a}$...

And similarly, $\frac{-\pi}{a}, \frac{-2\pi}{a}, \frac{-3\pi}{a}$…So, now only these points are the. So if we plot, the pattern is still parabolic. So, if we plot the parabola, this E k parabola, only these points on the parabola, will be the allowed k points, for the electron.

So, only these points will be the allowed k points, k equal to 0 is basically is not a physical point, because it belongs to or it signifies an electron that is not there basically. So, only these points on the parabola will be the allowed electronic states, for a when the electron is in the infinite potential well.

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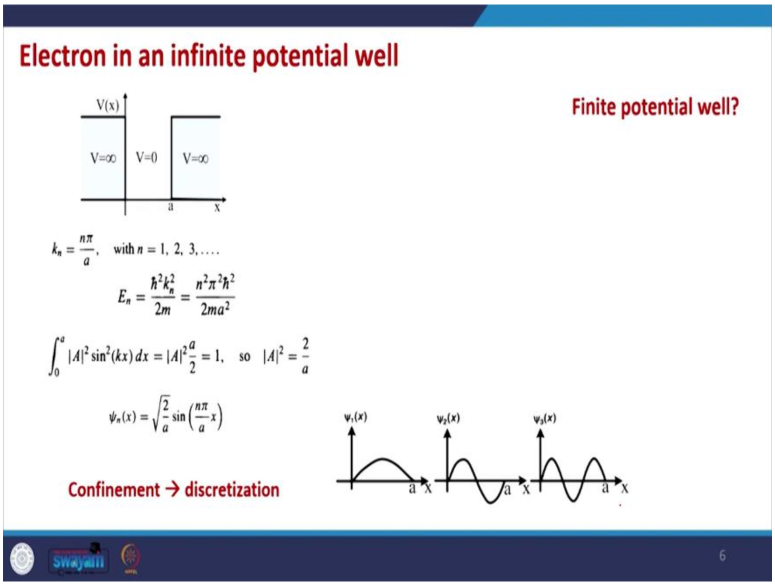

So, we have seen that when the electron is confined by a potential well, in that case, the systems energy are discretized and the E-k relationship gets altered. Now, we will extend the understanding of a free particle or free electron and electron in a potential well to electron in solids.

So, we will see now we have now since we have studied the free electron system and electron in a potential well, it will be quite natural for us to understand the electrons in solids, because solids are also in a way multidimensional potential wells, but they are not infinite potential wells, like the one that we studied. So, they are different kind of potential wells. And, the dynamics is more difficult or more complicated there and we will see that in coming classes.

Thank you for joining. see you in the next lecture.