Physics of Nanoscale Devices
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Lecture - 05
Electrons in Solids

Hello, everyone. Today, we will see how electrons behave in actual solids. Just to review what we have discussed so far.

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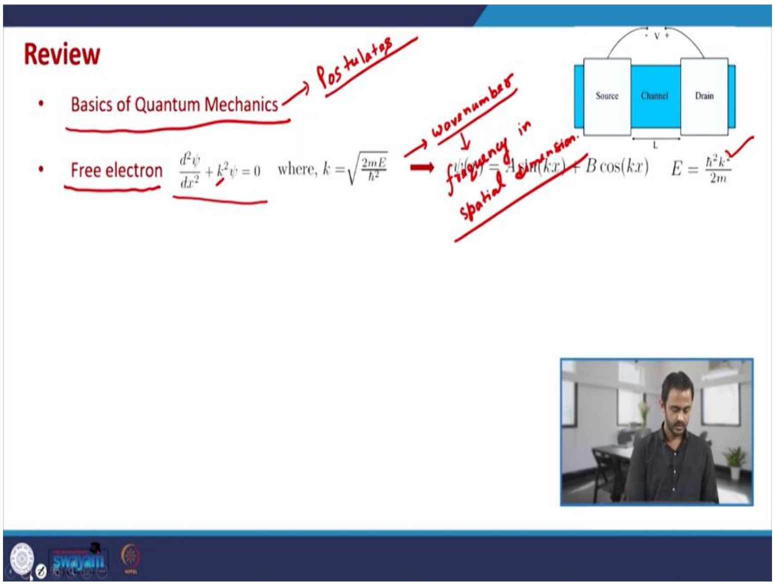

Review

- Basics of Quantum Mechanics → Postulates
- Free electron $\frac{d^2\psi}{dx^2} + k^2\psi = 0$ where, $k = \sqrt{\frac{2mE}{\hbar^2}}$ → wavenumber ↓ frequency in spatial dimension. ➡ $\psi(x) = A\sin(kx) + B\cos(kx)$ $E = \frac{\hbar^2 k^2}{2m}$ ✓

So, in the beginning I told you that the most important part of a device is of a field effect transistor is its channel. And the channel can be sort of understood as a two terminal device where we have a channel there is a source and there is a drain. And on application of a positive voltage on drain terminal electrons flow from source to drain. Now, as we know that in modern devices this channel region is getting smaller and smaller.

And now this channel region is nanometer in length and that is basically causing as we know and this we have already discussed. This is causing a fundamental change in the way electrons behave in the devices and that is what we are trying to understand in this course that is what we will be trying to understand in this course and that is what we have already that discussion we have already started.

So, ultimately in devices everything is basically the game of electrons everything is basically the dynamics of electrons how electrons behave in devices that is what we essentially need to understand in order to understand the physics of the device. And, in nanoscale nanoscopic devices when the channel region is few nanometers in length.

Electron's nature is no longer of a classical particle electron behave as a quantum particle and that is why we started our discussion with the basics of quantum mechanics. We discussed the basic postulates of the quantum mechanics and as you might recall some of the postulates of quantum mechanics are fundamentally different from the classical mechanics.

So, for example, in quantum mechanics we have a wave function to describe everything about a particle or a system. And we on doing measurement on a quantum system there is no deterministic result we get one of many possibilities as the outcome of the measurement.

So, quantum mechanics is fundamentally probabilistic whereas, the classical mechanics is a deterministic signs. We have also seen other postulates, how we define operators which correspond to physical observables in the system and after going through the basic postulates of quantum mechanics.

Now, after going through the basic postulates of quantum mechanics; we went on to understand the free electron how a free electron behaves. So, this is the first type in order to understand how the electron behaves in a solid. So, we started with how an electron behaves when it is entirely free, it is free from all the interactions all other kind of all other particles as if it is alone in the universe.

In case of free electron, we saw that the Schrodinger equation of the electron looks like a simple second order differential equation, where we have a parameter called k, which is also the known as the wave number just to sort of remind you a wave number can be understood as frequency in spatial dimension.

So, it basically tells how a wave or how a wave function is distributed in the space how it is oscillating how it is essentially repeating itself in the space. So, it is also known as the frequency in spatial dimension. And we saw that for a free particle case for a free electron when the electron is free from all the interactions, the electron wave function looks like a sinusoidal just a plane wave where the wave function is a superposition of sin and cosine.

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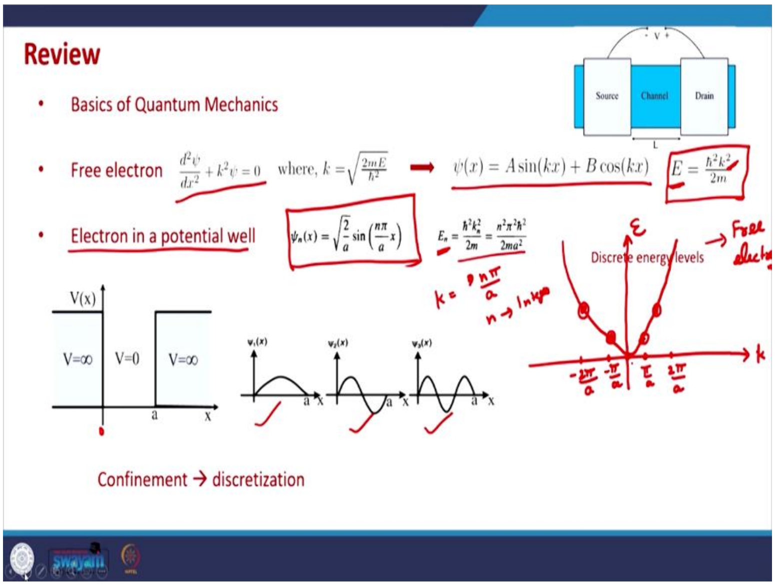

Review

- Basics of Quantum Mechanics
- Free electron $\frac{d^2\psi}{dx^2} + k^2\psi = 0$ where, $k = \sqrt{\frac{2mE}{\hbar^2}}$ ➡ $\psi(x) = A\sin(kx) + B\cos(kx)$ $E = \frac{\hbar^2 k^2}{2m}$
- Electron in a potential well $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$ $E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$

Confinement → discretization

And, in this case the relationship between the energy of the electron and the wave number of the electron is a parabolic relationship. So, for a free particle if we plot E k relationship, it is a parabola around E axis basically.

So, that is what we saw this is a simple solution a simple case of quantum mechanics which we can handle analytically. Generally, it happens that in quantum mechanics we cannot solve Schrodinger equation analytically precisely solve. So, we need to make many approximations.

But for free electrons, we can solve the Schrodinger equation analytically and this is how the solution looks like and this is the E k relationship for free electron ok. After free electron case, we try to understand how the electron would behave when the electron is confined in a potential well, what do we mean by a potential well?

Potential well has potential for has sort of potential boundaries between which between those boundaries the potential is 0 and in those boundaries beyond those boundaries the potential is infinite. So, what it means is that the electron is now confined between two points or two boundaries by a potential.

And in this case, we saw that, now the electronic wave function is still a sinusoidal wave function sinusoidal kind of wave function, but the energy values are no longer a continuous set of values. Now, the energy values are discrete values which are given as $E = \frac{n^2\pi^2\hbar^2}{2ma^2}$, which means that in a potential well, electrons can take only a certain set of energy values it cannot have any arbitrary energy and exist in the potential well.

It can only take certain set of energy values and corresponding to those energy values the electronic wave function will be defined by this equation and these are some of the simple wave functions corresponding to various energy values. And in this case, we saw that now if we plot the E k relationship for a particle in a box it will not be a continuous plot because the energy values do not exist for all k values the k can only take the wave number can only take $\frac{n\pi}{a}$ these values, where n is an integer.

So, the E k plot will be a discrete plot where the E values will still be lying on the parabola, but it will not be a continuous plot it will just be the points on this parabola like this. So, only these points will constitute the E k plot for a particle in a box. So, we consider two case one is the electron when the electron is entirely free and second case when the electron is entirely confined in a potential well.

And there are a range of intermediate cases there are lot of cases in between. For example, we can have a finite potential well, where this potential V is not infinite inside on the boundaries it is a finite value. So, V is no longer infinite. And in those cases, also, we can solve the Schrodinger wave equation and we can find out the electronic wave function, which will basically be like a hybrid of free electron and the electron in an infinite potential well.

Now, that key take away from this understanding was that when the electron is confined it leads to discretization and this was one of the earliest feature of quantum mechanics which was discovered and it was a paradigm shift in understanding of particles and their natures ok.

So, with this understanding, now we will see how electrons behave in solids basically. So, as you know as all of us know actually that solids can be quite complicated, they are not like free particle case or not like not even like particle in a box case they can be quite complicated.

Generally, the solids in devices that the solid that we use in devices are crystalline solids they are they have a regular defined lattice structure and, but still at finite temperatures those lattice points the solids and the lattice points might be vibrating and the solids might have many sort of non-idealities.

For example, there might be a lattice vacancy then the latest points are all vibrating. So, these kind of complications might be there in solids. So, we will not directly go into an actual solid actually because it is not possible to solve Schrodinger equation analytically for a for an actual solid for an actual lattice.

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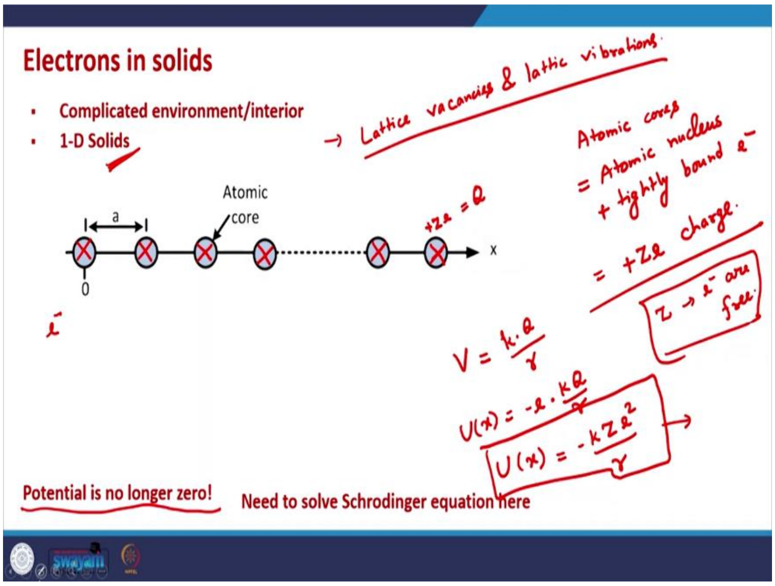

Electrons in solids

- Complicated environment/interior
- 1-D Solids

→ Lattice vacancies & lattic vibrations.

Atomic cores
= Atomic nucleus
+ tightly bound e^-
= $+Ze$ charge.

$Z \rightarrow e^-$ are free.

$V = \frac{k \cdot Q}{r}$

$U(x) = -e \cdot \frac{kQ}{r}$

$\boxed{U(x) = -\frac{kZe^2}{r}}$ →

Potential is no longer zero!

Need to solve Schrodinger equation here

So, what we do is we take the case of 1-D solids first 1-D solids and this case can easily be generalized to our 3-D solids and moreover in 1-D solids we do not consider lattice vacancies and lattice vibrations. So, we do not consider these two known idealities and we consider we first consider an ideal 1-D solid.

So, an ideal 1-D solid will look something like this. So, in an 1-D; in a 1-D solid the atoms or to be more precised the atomic cores will be located at a regular interval from each other. So, let us consider the case of an infinite 1-D solid in which these atomic cores, basically atomic cores are atomic nucleus plus tightly bound electrons. So, atomic cores are atomic nucleus plus tightly bound electrons.

So, the atomic cores and generally they have a +Ze charge. So, what it means is that in an atomic core a nucleus is there and some electrons are so tightly bound that we consider this entire system this atoms plus tightly bound electrons as one system, but Z number of electrons are Z number of electrons are free; which means that from each atom Z number of electrons are free to move in the entire solid.

So, that is why the atomic cores have a positive Z times e charge where e is the charge of a single electron. So, these atomic cores are positively charged stable atomic or stable heavy atomic cores basically. So, these are fixed at a regular interval the period of this lattice is let us say is a. Now, if an electron exist in this system, where there are there is a chain of atomic cores and we bring sort of one electron here.

So, we now we will try to see how an electron will behave in this particular system. And as we can see that in this system also like particle in a box system the potential is no longer zero; there will be some potential that the electron will feel because of the atomic cores, but just take a moment and think what will be the potential energy of the electron in this particular environment.

So, in this environment as you might recall the potential due to each atomic core will be a constant times the charge of the atomic core k times Q, Q is the charge of the atomic core which is basically Z times e in this case divided by r. And the potential energy of the electron would be the charge of the electron which is minus e times e into k Q by r.

So, the potential energy of the electron in presence of a single atomic core will be basically something like k times if we put the value of Q to be $\frac{Ze^2}{r}$. So, it is inversely proportional to the distance between the electron and the atomic core. And, if we plot this on corresponding to each atomic core, we will see how the potential profile looks like. So, corresponding to each atomic core the potential would be this basically inversely proportional to the distance between the electron and the atomic core.

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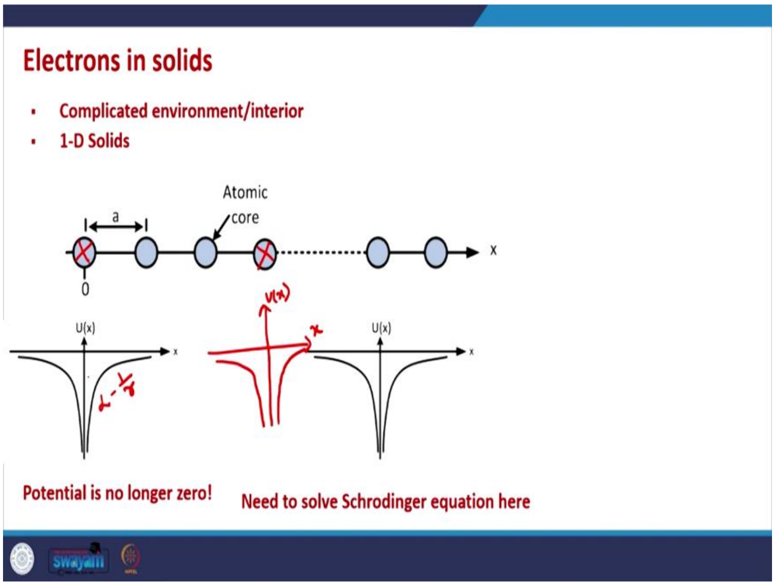

Electrons in solids

- Complicated environment/interior
- 1-D Solids

Potential is no longer zero!

Need to solve Schrodinger equation here

So, now let us see how it actually looks like potential due to atomic core due to let us say this atomic core is this as we can see this is basically the potential energy of the electron is inversely proportional to $\frac{-1}{r}$. So, the potential energy of the electron will be this, this is a graphical representation of the potential energy this is we are not.

In order to sort of have a good understanding of the nature of electrons we will sometimes use graphical representation of the system and their various parameters. So, the potential energy of an electron when it comes close to this atomic core will be this. And similarly, this will be the potential energy of the electron whenever it comes close to any of these basically any of these atomic cores.

So, we can individually say that corresponding to each atomic core in the lattice the potential energy of the electron will look like this. So, the resultant potential energy of the system would be basically a sum total of all these potential energies. So, that will be the final potential that the electron will see or electron will feel in this particular lattice. Let us see just for a for an exercise let us see how this potential energy looks like.

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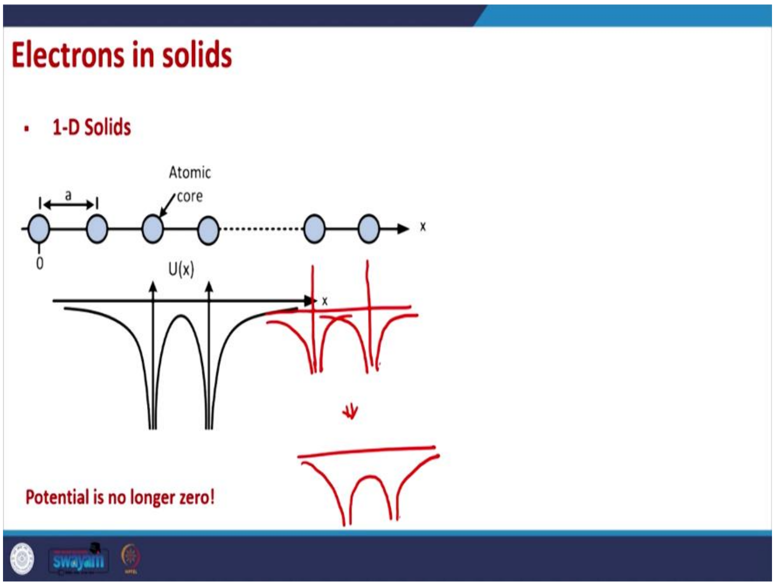

Electrons in solids

- 1-D Solids

Potential is no longer zero!

So, let us say if the potential energy due to this atomic core is this and potential energy due to this atomic core is similarly can be plotted to be this. So, the resultant potential energy of these two from these two atomic cores will be something like this. So, this is the resultant potential energy of the electron in presence of two cores, two atomic cores ok. And, similarly for a chain of atomic cores the resultant potential energy of the system would be like this, but extended to all the atomic cores ok.

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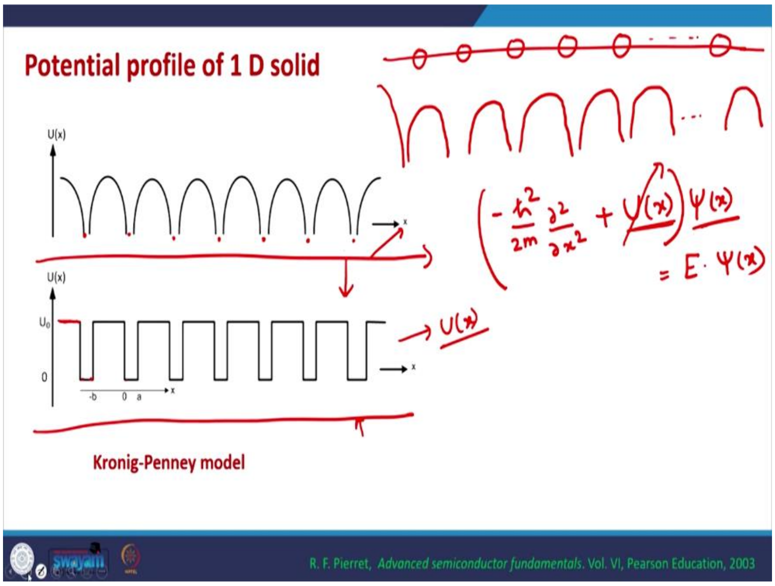

Potential profile of 1 D solid

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \cancel{V(x)}\right)\psi(x) = E\cdot\psi(x)$$

Kronig-Penney model

R. F. Pierret, *Advanced semiconductor fundamentals*. Vol. VI, Pearson Education, 2003

So, if we generalize basically this understanding this is how the potential profile or the to be more precise the potential energy profile of the electrons would be in a 1-D solid. So, in a 1-D solid if we precisely plot the lattice here the potential energy of the electron in this system would look something like this.

So, this is how the potential energy would look like. So, this is the potential energy of the electron in a 1-D solid and as you might recall the. So, ultimately, we need to we need to solve the Schrodinger equation for electron in any system in order to understand the nature of electrons or the behavior of electrons in that system.

And the Schrodinger equation looks like this in 1-D it would be $\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)$, where U(x) is the potential energy times the wave function equals energy of the electron times the wave function, ok. So, as you can see this parameter U(x) is quite important in solving the Schrodinger equation. So, if we need to understand the behavior of electrons in 1-D solid we need to put instead of in place of this U(x) we need to put this potential profile in the Schrodinger equation and we need to solve this Schrodinger equation.

And finally, the wave function that we will obtain will be the wave function of the electrons in this 1-D solid. So, that will basically capture all the information about the electrons in this solid. So, that is what we will try to do, but there is a cache here Schrodinger equation is not easy to solve always Schrodinger equation generally is difficult in most simple cases it can be solved.

But as soon as there are multiple atoms there is a complicated interaction between the atoms this it becomes difficult to solve the Schrodinger equation and that is also the case here with this potential profile if we take precisely this potential profile for 1-D solids we cannot solve the Schrodinger equation precisely.

But there is a way out here and this was given by Kronig and Penney and that is why it is known as the Kronig-Penney model. So, the technique that they use is that instead of solving the Schrodinger equation for this potential profile they sort of approximate or they solve the Schrodinger equation for a potential profile which is not exactly like which is not exactly the same as the potential profile of 1-D solids, but it resembles quite well with the potential profile of 1-D solids and this is the profile that the Kronig-Penney model takes.

And instead of having negative infinite potential energies at certain points which is the case at these points the Kronig-Penney model takes a finite value of potential energy at these points. So, in this particular figure it is taken to be as the reference point and the potential energy is considered to be zero at these points and the upper value of the potential energy is taken to be u naught.

So, this is not exactly the same profile as is there in 1-D solids, but this resembles quite well with the profile that is there in the 1-D solids and it turns out that this profile captures the most essential behavioral most essential characteristics of electrons in solids. So, if we solve Schrodinger equation for this profile in solids it will basically capture the all the essential components all the essential characteristics of the electrons.

So, that is why we solve the Schrodinger equation for the potential profile taken in the Kronig-Penney model and it turns out it also turns out that the Schrodinger equation can be precisely solved if we take U(x) to be this profile with some mathematical techniques. So, this is what we will do. In order to understand the nature of electrons the behaviour of electrons in solids we will solve Schrodinger equation for this potential profile the potential profile given in the Kronig-Penney model ok.

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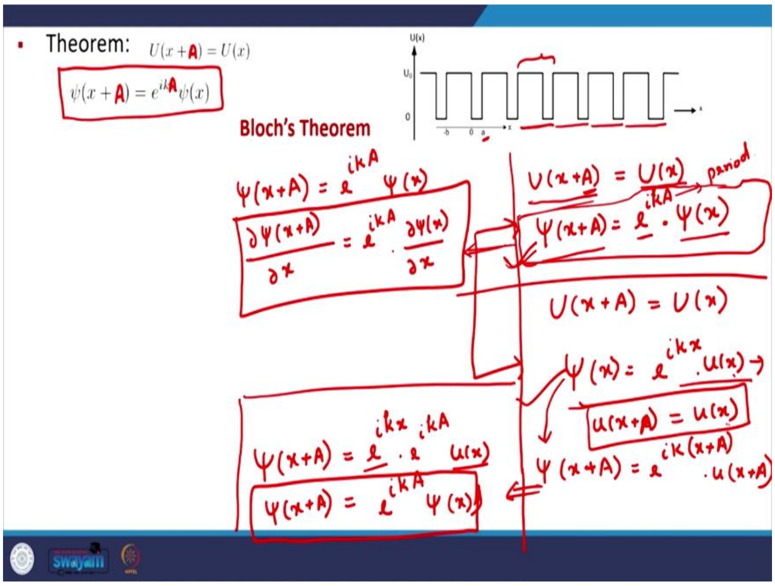

- Theorem: $U(x+\mathbf{A}) = U(x)$

$\boxed{\psi(x+\mathbf{A}) = e^{ik\mathbf{A}}\psi(x)}$

Bloch's Theorem

$\psi(x+A) = e^{ikA}\,\psi(x)$

$\boxed{\frac{\partial \psi(x+A)}{\partial x} = e^{ikA} \cdot \frac{\partial \psi(x)}{\partial x}}$

$U(x+A) = U(x)$ period

$\boxed{\psi(x+A) = e^{ikA} \cdot \psi(x)}$

$U(x+A) = U(x)$

$\psi(x) = e^{ikx} \cdot u(x) \rightarrow$

$\boxed{u(x+A) = u(x)}$

$\psi(x+A) = e^{ik(x+A)} \cdot u(x+A)$

$\psi(x+A) = e^{ikx} \cdot e^{ikA}\, u(x)$

$\boxed{\psi(x+A) = e^{ikA}\,\psi(x)}$

So, that is going to be our sort of next task again as you might have realized this is an infinite sequence of atoms in a 1-D the solid atoms can in principle be from minus infinity to plus infinity, but generally solids are finite in length, but the length can be extremely large on atomic scales.

So, for all practical purposes this can be taken to be quasi-infinite in length which means a huge number of atoms are there in the solids which means there are huge number of such patterns in the potential profile as you can see here. If you closely observe in this potential profile this particular pattern this pattern starting from here to here this is repeating itself for a large number of times for the entire length of the solid.

So, if we need to solve the Schrodinger equation for this entire solid essentially, we would need to solve the Schrodinger equation for all the for the entire length because the potential is changing it is as if there are there is a sequence of potential wells and or potential barriers in the solids.

And that is that in itself is also an extremely difficult task, but there is a rescue here I would say and the rescue is given by the so called Bloch's theorem. So, what Bloch's theorem says is that if a potential is repeating itself which means if there is a periodic potential then the wave function follows a certain pattern.

So, what Bloch's theorem says is that if a quantum system is in a periodic potential which means let us say let us take the period of the potential profile to be capital A because we are taking small a here. So, even in the statement of the Bloch's theorem let us take it to be capital A ok.

So, if the potential is periodic which means that after a period of capital A length the potential is again the same. Then the wave function will also be of this kind $\Psi(x + A)$, would be $\Psi(x). e^{ikA}$, the period where A is the period of the crystal.

So, in simple words or simply it can be understood that if the potential is periodic the wave function of the system will also be periodic, but modulated by an exponential ok or the restatement of the Bloch's theorem is that in a periodic potential which means if the potential profile is like this then the wave function of this system is e^{ikx}u(x). $\Psi(x)$ is e is e^{ikx}u(x), where u(x) is a periodic function ok.

So, these are these two statements of the Bloch's theorem are equivalent and we will see here. So, in this expression if we put Ψ instead of x if we take $\Psi(x + A)$ it will basically be $e^{ik(x+A)}$u(x+A) and as we know u(x+A) is essentially u(x) because u(x) by definition is a periodic function.

So, this $\Psi(x+A)$ would basically be $\Psi(x+A)$ would be e^{ikx} let us also decompose the exponential u(x). So, in place of u(x+A) we can put u(x) in this expression and e^{ikx}u(x) is basically $\Psi(x)$ as is clear from this equation. So, $\Psi(x+A)$ would be $e^{ikA}\Psi(x)$ which is essentially the earlier statement of the Bloch's theorem this statement of the Bloch's theorem.

So, the Bloch's theorem can equivalently be put in two statements in a periodic potential profile the wave function of the system would be $\Psi(x+A)$ equals $e^{ikA}\Psi(x)$ or $\Psi(x)$ can be written as $\Psi(x)$ equals e^{ikx}u(x) where u(x) is a periodic potential which means u(x+A) is the is same as u(x) ok.

So, these are two equivalent statements of Bloch's theorem we will not be going into the derivation of the Bloch's theorem in this class, but I would highly recommend you to go through the derivation of the Bloch's theorem which is available in many standard texts on solid state physics and condensed matter physics. This is an this will be an interesting exercise this will clear many quantum mechanical concepts as well building on Bloch's theorem.

So, I am taking a detour in order to go into the details of Bloch's theorem here this also means this statement of Bloch's theorem means that this statement $\Psi(x+A)$ equals $e^{ikA}\Psi(x)$ this means; if we take the first derivative of Bloch's theorem it would basically be $\frac{\partial\Psi(x+A)}{\partial x} = e^{ikA}\frac{\partial\Psi(x)}{\partial x}$.

So, these two statements of Bloch's theorem are equivalent to each other. So, in other words the Bloch's theorem can be stated in terms of psi x plus A which naturally implies that the same expression holds true for the derivative of the wave function as well ok. So, there are two statements of Bloch's theorem this one and this one and as we have seen these two are equivalent statements and the implication of this statement is that the derivative of the wave function can also be represented in the same form.

So, today what we have seen is that the interior of solids or the potential profile in solids is slightly complicated. And we need to make some approximation in order to sort of solve the Schrodinger equation inside the solids and that approximation was done in Kronig-Penney model of electrons in solids.

And there also we cannot just take the potential profile and solve the Schrodinger equation there also we need to invoke Bloch’s theorem and in next class ,in next lecture we will see how by using Bloch’s theorem we can solve we can analytically solve Schrodinger equation in 1-D solids with Kronig- Penney approximation.

Thank you and see you in the next class.