Physics of Nanoscale Devices
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Lecture - 07
KP Model, Effective Mass

Hello everyone, today we will conclude our discussion on KP Model and if time permits we will also discuss the notion of Effective Mass. Before going into these ideas let us see what we did in last couple of classes, last couple of discussions and as you might recall, we were discussing how an electron behaves in actual solids.

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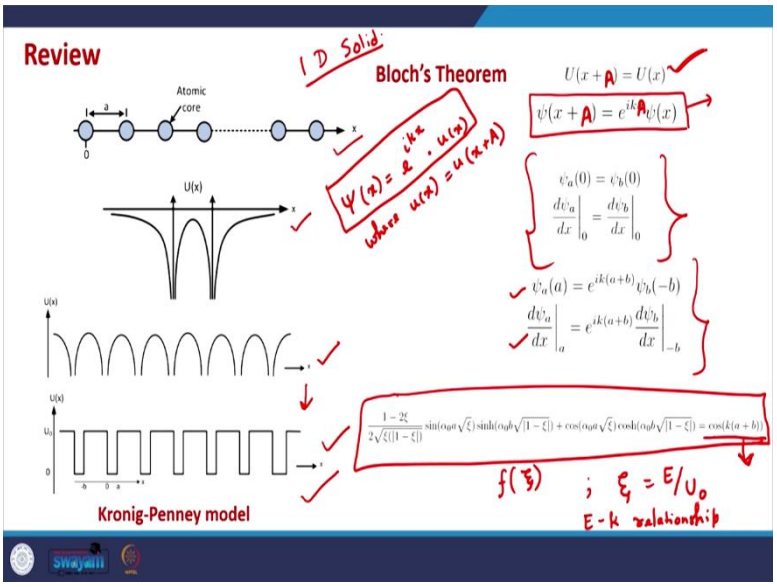

And we considered the case of 1D solid and a 1D solid has atomic arrangement or to be more precise atomic cores arranged in this way. And the potential profile, the potential energy of the electron due to two of these cores will look like this and the potential energy of the electron because of the entire chain of atoms, because of the entire 1 D solid will look something like this.

And this is with this potential energy we need to solve the Schrodinger equation in order to precisely determine the behaviour of electrons ok. And here we invoked the Kronig-Penney model the KP model so called KP model which allows us to solve the Schrodinger equation for electrons in 1D solid precisely.

But with a slightly different kind of potential profile, here we avoid infinite infinities in the potential energy and we take finite potential energy values and the profile looks pretty much similar to what it is there in the actual solid not exactly same, but quite similar to that.

And with this potential profile we saw that by using Bloch's theorem which essentially allows us to calculate the electronic wave function when we have periodic potential; by using Bloch's theorem we can solve for the Schrodinger equation in the KP model potential energy. And this is what we were doing, we were after solving the Schrodinger equation we used boundary conditions and there are and there were four unknowns in the Schrodinger equation.

Two equations actually and there were four unknowns and we used four boundary conditions and two of these boundary conditions come from the continuity of the wave function and continuity of the derivative of the wave function and the two other boundary conditions come from the statement of the Bloch's theorem. The statement of Bloch's theorem about the wave function and the statement of Bloch's theorem about the derivative of the wave function.

So, this is the so, given a periodic potential this is the statement of the Bloch's theorem and equivalent statement of Bloch's theorem is that in a periodic potential, the wave function can be written as like a plane wave $\Psi(x)$ is plane wave multiplied by a periodic function where u(x) is a periodic function which means u(x) is u(x+A) where A is the period of the potential energy ok.

So, these two statements of Bloch's theorem can be used interchangeably and what we also observed here is that this parameter k comes from the Bloch's theorem and it is the so called crystal momentum of the electron ok. So, after solving these four boundary conditions after solving for the coefficients in Schrodinger equation from these four boundary conditions we finally, came up with this constraint or this equation, the solution of this equation will give us the values of energy corresponding to a k value ok.

So, on the left hand side we have a function which is which we have a function where the parameter is ξ. So, on the left hand side there is a function of ξ where ξ is essentially E/U_o where E is the energy U_o is the potential from the Kronig- Penney model. On the right

hand side we have a cosine function and the cosine function has k in its parameter basically cosine of k into (a+b) ok.

So, on the left hand side we have energy function on the right hand side we have the k function the crystal momentum function. So, in essence it will give us the energy corresponding to a given value of k ok. So, it will give us the E k relationship for the solids in particular 1D solid.

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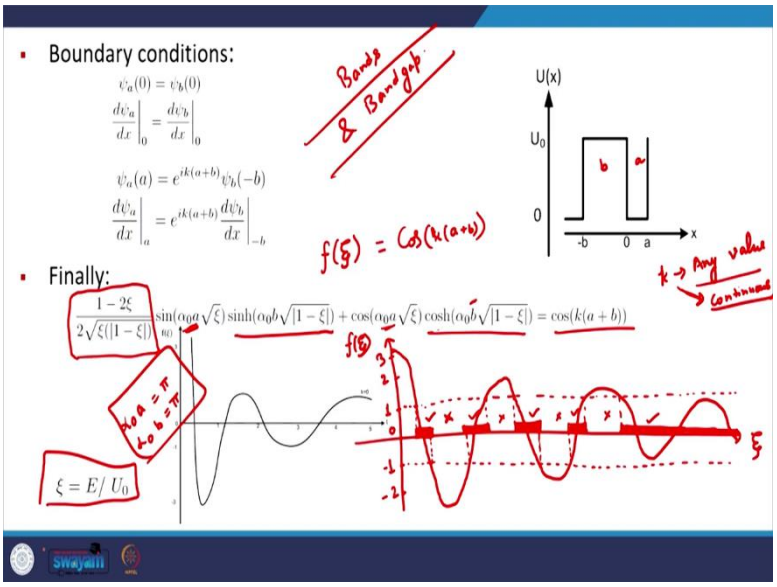

So, that is what we will see and we will try to understand that. So, as I told you in the previous class as well. Now, because of the Bloch's theorem by virtue of the Bloch's theorem we just need to solve Schrodinger equation in one period of the potential in two regimes, regime a and regime b and by using Bloch's theorem we could solve the Schrodinger equation and finally, this is the constraint that we came up with.

So, on the left hand side we have a function which has coefficients as xi parameters xi and there is this hyperbolic terms as well. So, the mathematical solution would be slightly complicated would be complicated. In fact, it would take a lot of time to do the exact mathematical solution of this equation.

So, that is why we resort to the graphical representation of the solution. And what we do is we plot $f(\xi)$ which is essentially the left hand side function as a function of ξ, ok and

as you might have already realized that in order to plot this $f(\xi)$ function we also need these parameter values, these system parameter values.

So, to say these α_oa values for example, α b value. So, these α_o, a, b these three values we at least need to have. So, for a standard for a standard value of let us say α_oa let us take it to be π and or we can take any arbitrary value of these constants and then if we plot this function $f(\xi)$ as a function of ξ, it will be something like this it will be a hyperbolic function.

Hyperbolic means that initially the amplitude is high its starts with a high amplitude, but gradually the amplitude decays. So, gradually this is how this function typically would look like. So, this is the plot of the left hand side function and as you might have already realized that on the right hand side, we have a cosine function cos k into a plus b and for an infinite crystal for an infinite solid this k can take any value.

So, basically k will have continuous values. So, which means this right hand side function for an infinite 1D solid will be a function oscillating between plus 1 and minus 1 this can take any arbitrary value between plus 1 and minus 1 on the right hand side.

On the left hand side however, we have an we have a hyperbolic function which can take values from which initially has high amplitude, but the gradually the amplitude decays down. So, the E and k values which will jointly satisfy this equation if we try to figure that out from this plot; those values will be those values of energy or those values of this parameter ξ which will make or which will for which this left hand side function is between plus 1 and minus 1.

So, what I mean is that for those values of ξ for which this lhs function left hand side function is between plus 1 and minus 1 for those values of xi we will have a valid k value.

Because, the right hand side function can only take values between plus 1 and minus 1 it can only go from plus 1 to minus 1. So, those values of xi which makes the left hand side function greater than plus 1 or less than minus 1, they will not have any value any k value corresponding to them. So, what it means is those energy values will not have any k value corresponding to them which means those energy values are not permitted for the electrons.

Electrons cannot occupy those energy levels that is the physical intuition behind the solution of this equation. So, let see it here we have now plotted dotted lines between plus 1 and minus 1 and we now see that on the ξ axis in this range of ξ values and similarly, in this range of ξ values the left hand side function is between plus 1 and minus 1. Similarly here between these values of ξ also between these values of ξ.

So, this is not an exact plot, but this is a qualitative picture how the solutions of the Schrodinger equation exist according to the KP model and we can see that there are certain ξ values which in other words mean. There are certain energy values for which there exist a valid k which means there exists a valid wave function and there are certain other energy values for which there is no valid k which means there is no valid wave function corresponding to those ξ values.

So, these highlighted portions on ξ axis essentially are the ξ values for which we have a valid k value, we have a valid crystal momentum for the electron. So, we can say that the electrons will occupy or electrons can only occupy these energy values and there are certain energy values which are prohibited for the electron, you might now correlate it directly to the idea of the bands and band gap which most of you might already be familiar with.

In solids we have allowed energy bands where the electrons can occupy valid states or we have a certain range of energy where electrons can take or electrons can take those energy values and in band gap the electron cannot exist electron wave function cannot exist. So, those are the disallowed energy values for the electron in solids and here also we can directly see that there are certain values of ξ which are permitted for the electron and there are certain values of ξ which are not permitted for the electron.

So, these permitted values in other words are the energy bands the allowed energy bands and these ξ values where the electron cannot exist these are the band gaps. So, similarly we can see it on the entire ξ axis ok. So, if you recall our last few classes a free particle when the electron is totally free it is not interacting with anybody in the universe or it is as if it is the only thing in the universe, electrons energy is continuous it can take any energy value when the electron is confined in a potential well, it can only take discrete values ok.

But now, the potential profile is slightly complicated. Potential profile is periodic and in periodic potential profile electrons can takes certain range of energy values and they are not allowed to take certain other ranges of energy values and these are called the bands, energy bands and band gaps in a solid. So, the notion of bands and band gaps come directly from the solution of the KP model solution of the Schrodinger equation according to the KP model ok.

So, that is actually the advantage of understanding the KP model it very clearly explains how the notion of bands and band gaps arise in the solids ok. So, with this understanding we will go a little bit deeper now, in order to understand how the electron actually behaves in solids.

There are few other points this is a slightly better plot of $f(\xi)$ as a function of ξ and as you can see here, it is clearly mentioned when we plot $f(\xi)$ as a function of ξ this function takes hyperbolic value and there are certain energy values which are allowed for the electron as is also clear in this plot ok.

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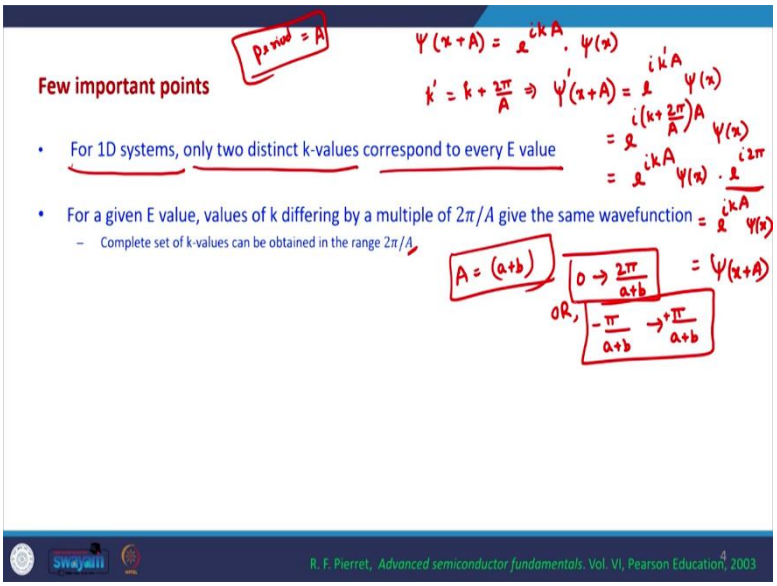

So, with this understanding there are few other few more important points that we need to keep in mind, while trying to understand electrons in solids and those points have not been mathematically derived here, because of the lack of time I would say and lack of and we did not intend to cover that in this course, but please keep those things in mind and if you

have time please go through the derivation of Bloch's theorem and these things will become quite obvious.

Or these these things will naturally come from the solid derivation of the Bloch's theorem ok. So, a few important points that we need to keep in mind is that for 1D systems only two distinct k values correspond to every energy values. So, in 1D solids for every energy values there are two k values which will give that energy value ok. So, if we go back to this constraint for every ξ value there will be two k values which will give us the a valid ξ value ok.

Second is if the period of the potential profile is A if the period of potential is capital A then the k values the values of k which differ by a multiple of $2\pi/$A. This capital A they give the same wave function for the electrons basically or in other words the k values which are separated by $2\pi/$A, they essentially give the same wave function and that is a direct consequence of the Bloch's theorem.

Because if we look back to the Bloch's theorem, Bloch's theorem states that $\Psi(x + A)$ is essentially $e^{ikA}\Psi(x)$. So, this is the standard statement of the Bloch's theorem and so, instead of k if we take k' to be k + $2\pi/$A and we put this value of k' in this equation. And let us say the wave function now is Ψ', is $e^{ik'A}\Psi$(x) and if you put k' to be k + $2\pi/$A.

So, this will essentially be e^{ikA} times Ψ(x) into $e^{i2\pi}$ which is essentially one this is one. So, this turns out to be $e^{ikA}\Psi(x)$. So, which is $\Psi(x + A)$. So, a k value shifted by $2\pi/$A gives the same wave function essentially ok. What it means is that the complete set of k values is now in the range of $2\pi/$A or -$\pi/$A to $\pi/$A ok.

So, the complete set of k values complete set of k values exist in the range of $2\pi/$A, where A is the period of the potential profile in our KP model discussion the potential of the period of the potential profile was small a plus b in that case capital A was a+b. So, all the valid k values or complete set of k values will be between 0 to $2\pi/$(a+b) or -$\pi/$(a+b) to $\pi/$(a+b) ok.

And this is an important statement please keep this in mind. This has a simple derivation as well this is also clear from the mathematical form of the Bloch's theorem.

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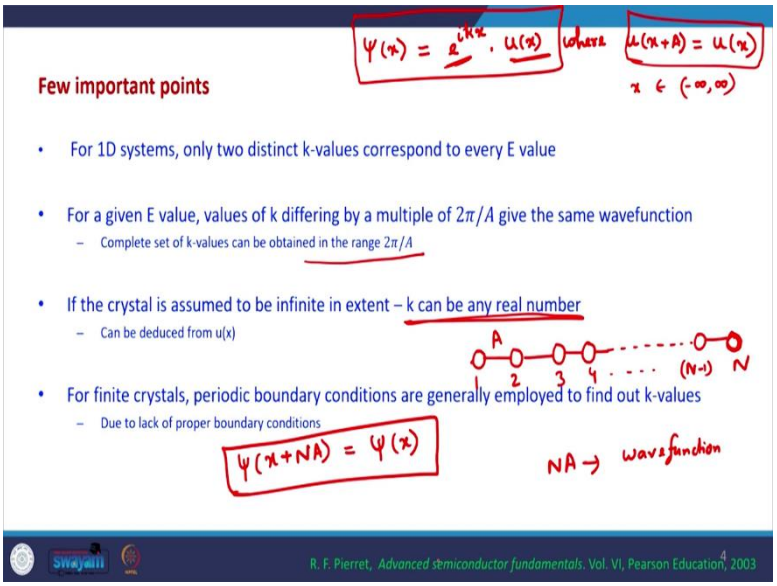

The third point that we need to keep in mind is that if the crystal is assumed to be infinite in extent, in that case this k can be any real number. So, if the crystal is infinite or very long as compared to the dimensions as compared to the distance between two atoms in that case k can take any real number and there is no other constraint on k.

And this we can see also from the statement of the Bloch's theorem the statement of the Bloch's theorem says that the wave function can be written as $e^{ikx}u(x)$, where u is a periodic function with the period of potential profile ok. This is the another this is sort of another statement of Bloch's theorem which we have discussed many times and if the crystal is infinite in extent which means this x can go from minus infinity to plus infinity.

It can go from minus infinity to plus infinity in that case u(x) will be well defined, because u(x) is a periodic function it will be well defined over all the places. If it is well defined in one period because of this virtue, because of its periodicity a periodic function is everywhere. So, the only thing that needs to be well defined is this plane wave solution or this e^{ikx} term and this will be well defined, if k is a real number.

Because, if k becomes an imaginary number in that case this exponential will blow up at infinities ok. So, if the crystal is extremely large as compared to the distance between two atomic cores, in that case k can be any real number. Another constraint is k can take values or complete set of k values can be obtained in the range of 0 to $2\pi/$A.

In other words it also means is that if two k values are shifted by or 2 k values are located by $2\pi/A$ distance from each other then the wave function corresponding to these two k values will be the same. Another point is that for finite crystals generally this is just to keep in mind, when the crystals are finite which is actually the case in most of our devices we invoke what is known as the periodic boundary conditions.

Because, practically speaking we do not have proper boundary conditions on the boundaries of the crystal boundaries of our device and this periodic boundary conditions give good approximation to the actual scenario. So, what is the periodic boundary condition? So, in a finite crystal which means that now the crystal has N number of atoms 1 2 3 4 up to (N-1), N number of atoms, atomic cores and if the distance between each of them is A.

Then what we assume is that the wave function here, periodic boundary condition means that this is the period of the this N times A, the entire length of the crystal is the period of the wave function. What it means is that the wave function at this end of the crystal this end of the solid and this end of the solid will be the same. What it means mathematically is $\Psi(x + NA)$ is equal to $\Psi(x)$.

So, this is the periodic boundary conditions and for all practical purposes it gives good results by results I mean the valid k values. So, if we sort of do slight analysis here.

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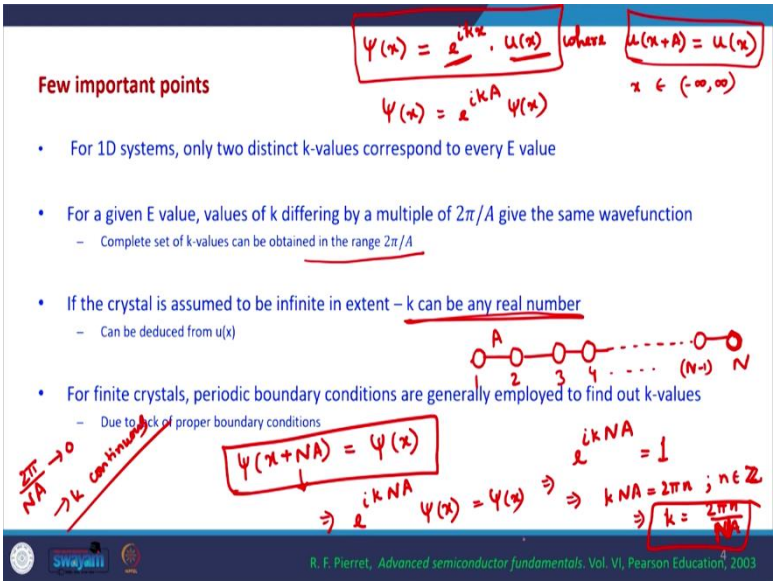

What this implies is from the Bloch's theorem we can say $\Psi(x + NA)$ would be from this statement of the Bloch's theorem $\Psi(x + NA)$ would be e^{ikNA}. $\Psi(x)$ would be equal to $\Psi(x)$ because of the according to periodic boundary condition NA is also the period of the potential profile.

So, the Bloch's theorem can be applied here as well and what it implies is that e^{ikNA} is 1, which basically means that kNA would be 2πn where n can be any integer. So, k is basically 2πn/NA. So, the for finite crystals k will have discrete values and these discrete values will depend on the length of the solid or length of the crystal itself NA the distance between two atoms and there this will be 2πn/k. k values will be separated by 2πn/NA and this small n is can be any integer.

And we can also see from here, if this capital N is extremely large as compared to small n then this will be almost a continuous set or sorry if capital N is very large number, in that case the distance between 2 k points will be almost 0. So, which means that k will be continuous; k can take any continuous values as we have already discussed in our previous slide.

So, these were few more important points apart from the idea of the energy bands and band gap that arises out of the solution of KP model. These are few other points that we need to keep in mind, while sort of trying to understand the electrons in solids.

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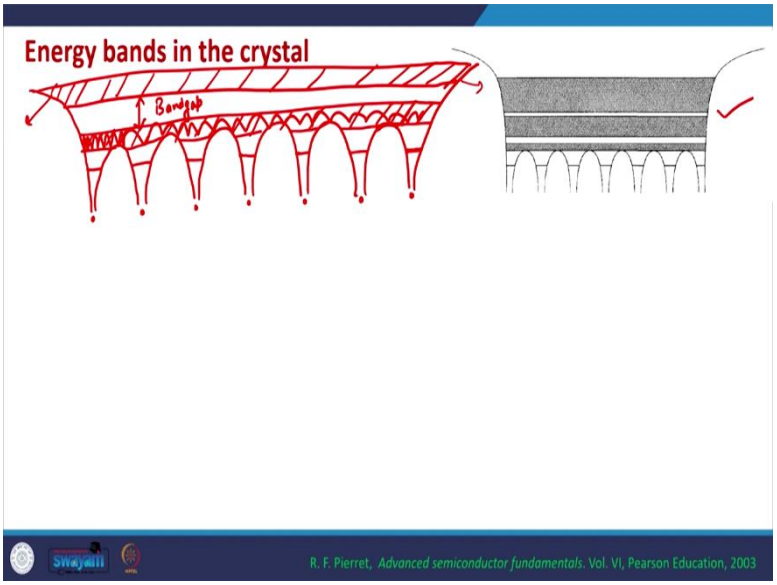

So, now extending our discussion of energy bands, generally it is the case that the energy bands the notion of energy bands is not mathematically clear to most of us. But it is not intuitively or physically clear in our minds and this is what we will try to see here, this is by no means is an actual plot, but this is how the bands look like in a solid.

So, as we have already seen that the potential profile in a solid looks something like this. These are the this is the potential energy of electron in a solid ok. Here are the atomic cores and as we had already seen close to the atomic course the potentials the potential energy of electrons go to negative infinity ok.

So, this is what we started with these are the ends of the solid and by making an approximation using KP model we solved the Schrodinger equation and we saw that there are certain energy values, which the electron can take and there are certain other energy values which the electron cannot take ok. So, if we picture that here in this particular potential profile, let us say if this energy value is allowed we will have a range of energy values which are disallowed.

So, for example, energies between this and this will be these two levels will be disallowed. So, we will have this energy range which will be allowed. So, if the energy of the electron is less than this u naught value, this was the u naught value it will have a discrete energy level almost a discrete energy level.

If the energy of E the energy of electron E is greater than U_o which is the peak of the this potential period, in that case there will be a range of energy values which is allowed and there will be a range of energy values which will be disallowed. So, these are the allowed energy values or this is a valid electronic band in the solid and these are the this is the another band, another range of energy values allowed and in between this is the disallowed range or the band gap in the solid as is pictured here ok.

So, this is the physical picture corresponding to the potential profile in a solid, physical picture of energy values of electrons in a valid energy values in a solid, in a 1D solid particularly ok. So, this brings us to the notion of Brillouin zone which we will discuss after this and I will discuss that in the next class, because that might take some more time. But I hope that in this class how the bands and band gap arises in solids that is now mathematically and intuitively clear to us.

Thank you for your attention, I will see you in the next class.