Introduction to Quantum Mechanics
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Lecture - 02
Solution of the Schrodinger equation for one-dimensional periodic potential: Bloch's theorem

So, far we have discussed a couple of examples of solving the Schrödinger equation in different potentials.

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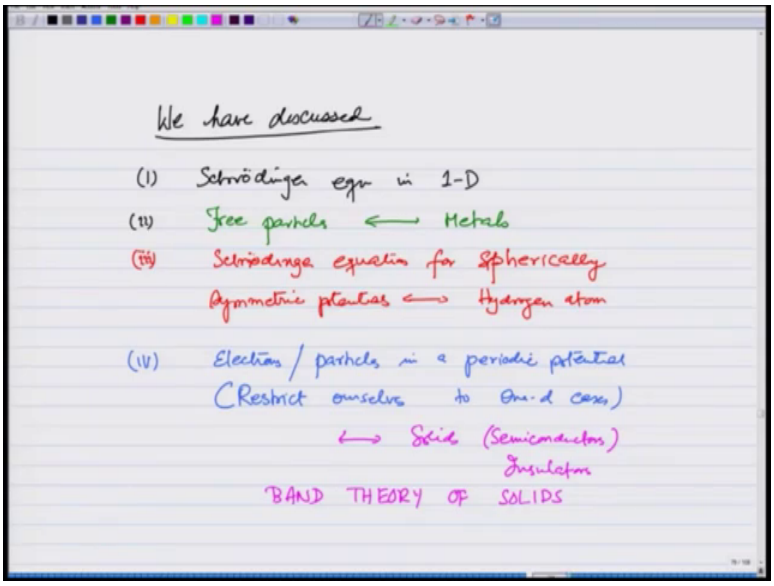

So, we have discussed one Schrödinger equation in 1D. Then we have also discussed free particles and this was related to metals. We have also discussed Schrödinger equation for spherically symmetric potentials. And this was related to hydrogen atom or hydrogen like ions, and this lecture on word and this is the final example that we will be doing in this course. We are going to focus on electrons or particles in a periodic potential and again we will restrict ourselves to one dimensional cases. And that is sufficient to give you an idea how bands arise and this would be related to solids. In general metals are also like this and in particular semiconductors and insulators can be explained through this electrons being considered in a periodic potential, and what gives rise to is the band theory of solids.

So, let us see what is, so specific about periodic potentials.

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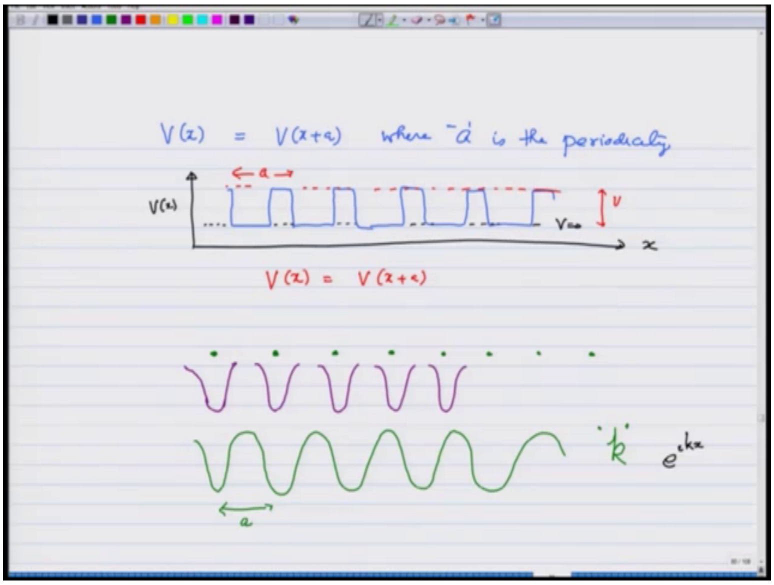

So, when I talk about a periodic potential in 1D v x this is v x plus a, where a is the periodicity. Let me explain this by making pictures. So, for example, if I have a potential like this, where I have shown the potential energy along the y axis and x is; obviously, on the horizontal axis. And let us say this level which I am showing through dotted lines is v equals 0 and the height of the potential which I am showing by the red dotted line is v. Then you see after a certain distance the potential repeat itself. So, this is the period a.

So, this potential v x is equal to v x plus a, this is a very simple example. We can also have for example, one dimensional atoms separated by equal distances going all the way from minus infinity to infinity. So, these are the atoms which are shown by green dots in 1D, and each one has it is own potential. So, let me make that potential like this and let us say for proper description I make it finite at the position of the one dimensional atom and this repeats is the same everywhere. Finally, when I add all these potentials what I get is the potential like I am showing in green out here like this. And it has a period of the distance between the atoms. So, this is also a periodic potential.

And we want to solve the Schrödinger equation in this the periodicity of the potential makes a solution simple as well as it gives me a new quantum number k. Recall that for free electrons I had the solution e raise to i k x, where k was related to momentum here also I am going to have a quantum number k, but please do not go by the similarity in the notation k does not represent the momentum in this case as we will see.

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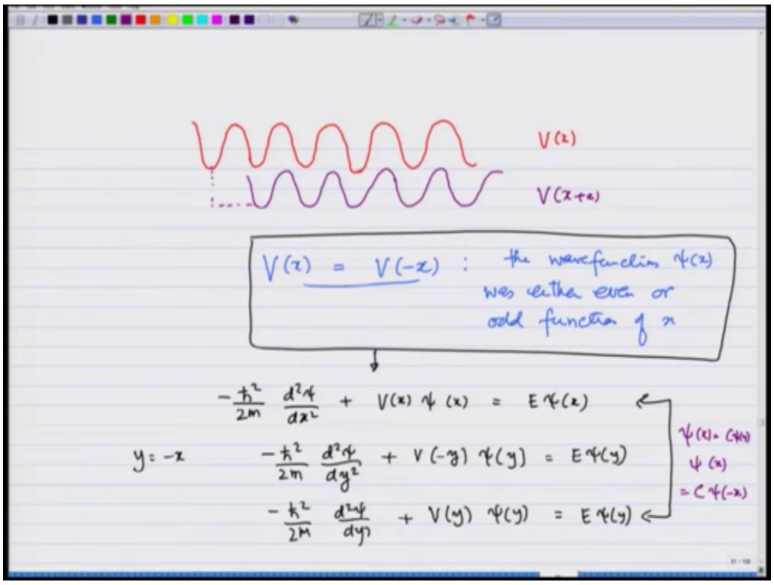

So, whenever there is a symmetry in this potential let me make it like this the symmetry is that if I displays the whole thing by a; that means, I shift suppose this point by a. So, this thing looks like this. You cannot really distinguish the shifted system from the original system right. So, v this is v x plus a and the red one v x this is a cemetery recall earlier we had encountered a symmetry in the cases where v x was equal to v minus x. And in that case we showed that the wave function psi x was either even or odd function of x.

So, symmetry led to this property as wave function. Similarly it is this symmetry out here. That the system looks exactly the same when we shifted by a or the periodicity is going to lead to certain property as wave function which is described by a theorem called Bloch's theorem. To motivate Bloch's theorem let me recall again how did we arrived at this conclusion for the potential which was symmetric about x equals 0.

So, in this case Schrödinger equation is minus h cross square over 2 m, d 2 psi over d x square plus v x psi x is equal to E psi x and what we did in that case was we replaced x by minus x. So, we wrote x y equals minus x and therefore, the equation in terms of minus x became minus h cross square over 2 m d 2 psi over d y square plus v minus y psi y equals E psi y. And therefore, the equation became minus h cross square over 2 m d 2 psi over d y square plus v minus y is the same as y v y psi y equals E psi y.

Notice that the 2 equations are exactly the same. So, they have the same solution and therefore, at most the solutions could differ by a constant. So, we had psi x equal sum constants psi y or we had psi x equals sum constant psi minus x. Since mode psi square remains same because the system has remain the same, when I switch or turned it around by pi. C could be either plus 1 or minus 1 that led to the conclusion that the wave function should be either an odd function. Or an even function we are going to do now exactly the same thing in this periodic system.

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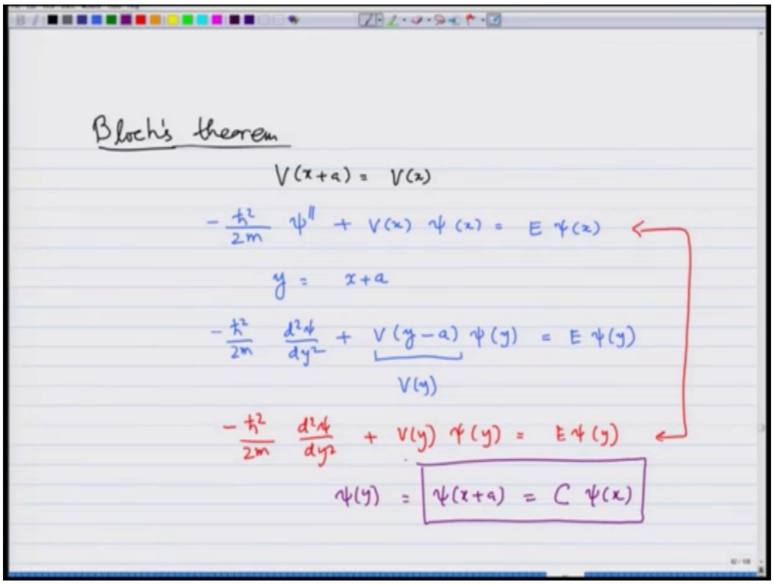

So, I am going to now discuss something called Bloch's theorem in which case v x plus a is the same as v x. So, my Schrödinger equation is minus h cross square over 2 m psi double prime plus v x psi x equals E psi x. Let me write y equals x plus a, then I have minus h cross square over 2 m d 2 psi over d y square because the derivative would remain the same even if I shift the coordinate by a, plus v y minus a psi y equals E psi y. Now v y minus a is the same as v y and therefore, this equation is minus h cross square over 2 m d 2 psi over d y square plus v y psi y equals E psi y.

Now, these 2 equations are exactly the same. So, at most I could have is that psi y which is psi x plus a would be equal to sum constant psi of x, this is the conclusion.

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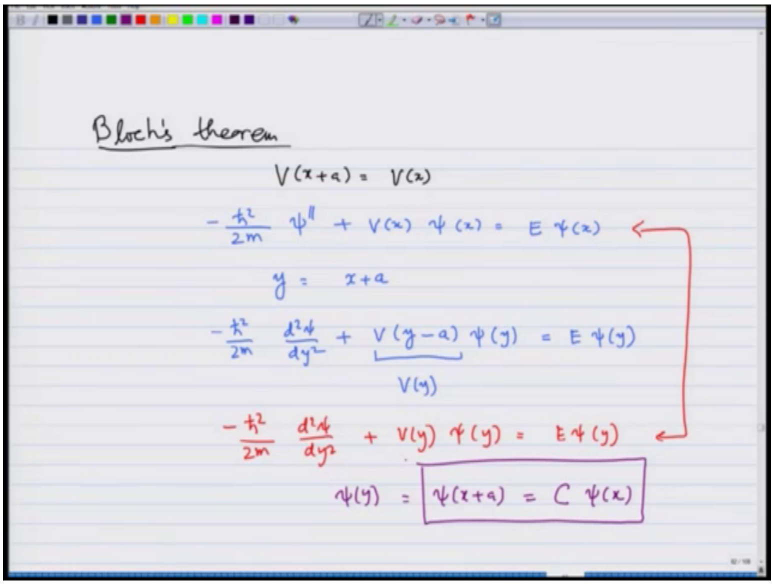

Now, I can do it one more time. So, I can now right my original equation was minus h cross square over 2 m. D 2 psi over d x square plus v x psi x equals E psi x. And take y to be equal to x plus 2 a. So, even if I shift the system by 2 a nothing really changes. So, again I am going to have the equation minus h cross square over 2 m d 2 psi over d x square plus v y minus 2 a which is again the same as v y sorry this should be y square psi y equals E psi y is exactly the same equation. So, I am going to have psi y equals sum c 2 because I have shifted by 2 psi x. So, remember now if we shift the lattice or the potential by a I get psi y equals c 1 psi x and if we shift the lattice by 2 a I get psi y equals c 2 psi x.

Now, think of this that if I shifted lattice one by one I would have gotten if 2 a shift was done a step at a time, then I would have gotten psi in the second case to be c 1 square psi x. And this implies the c 2 is equal to c 1 square that is conclusion number 1.

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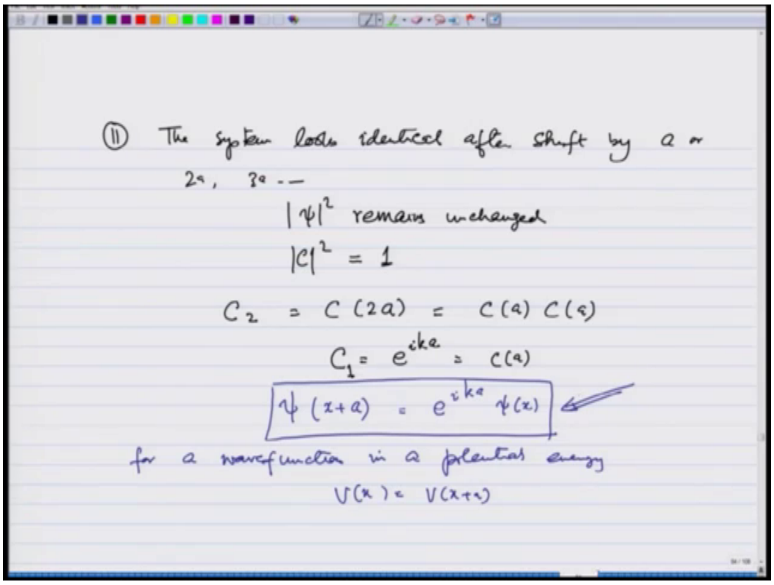

Conclusion number 2, the system looks identical after shift by a or 2 a or 3 a or so on.

And therefore, mode of psi square remains unchanged. Probability of finding a particle at a particular point should remain unchanged, if I shift the system because is it is infinite system and therefore, mode c square whether it is c 1. Or c 2 or c 3 is equal to 1. So, I have c 2 which is represented let us say by c 2 a shift by 2 a is equal to c a c a and modulus of each is the same and therefore, the only choice I have is write c as sum e raise to i k a c 1 which is c a. Has satisfy both the properties, and therefore I am going to have psi if I shift by a is going to be equal to e raise to i k a psi of x, for a wave function in a potential energy v x equals v x plus a.

So, if a particle is moving in a periodic potential this is the property that it is going to satisfy.

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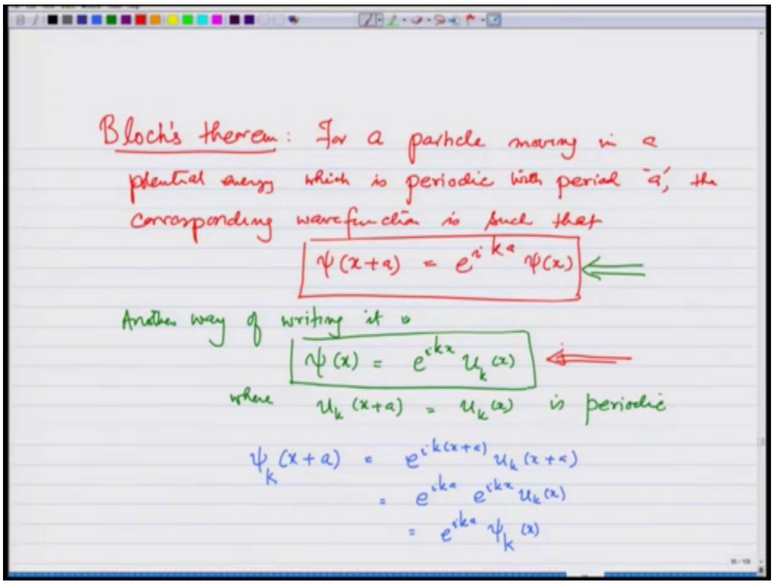

So, let us write this Bloch's theorem for a particle moving in a potential energy which is periodic with period a the wave function, is such that psi x plus a is equal to e raise to i k a psi x. That is the Bloch's theorem. Another way of writing the same thing of writing it is that the wave functions psi x is equal to e raise to i k x sum u k x, where u k is periodic with the same periodicity is periodic. This automatically satisfies the upper property, how so? So I am going to have psi x plus a equals e raise to i k x plus a u k x plus a. And since u is periodic I am going to have this as e raise to i k a e raise to i k x u k x which is same as e raise to i k a psi, let me now label it as k x let me now label this as k x.

So, both are the same properties. So, this is the Bloch's theorem that the wave function in a periodic potential, this is a Bloch's theorem. That a particle moving in a periodic potential has the form of the wave function which is given either by this upper box or the lower box both are one and the same thing. This leads to interesting properties.

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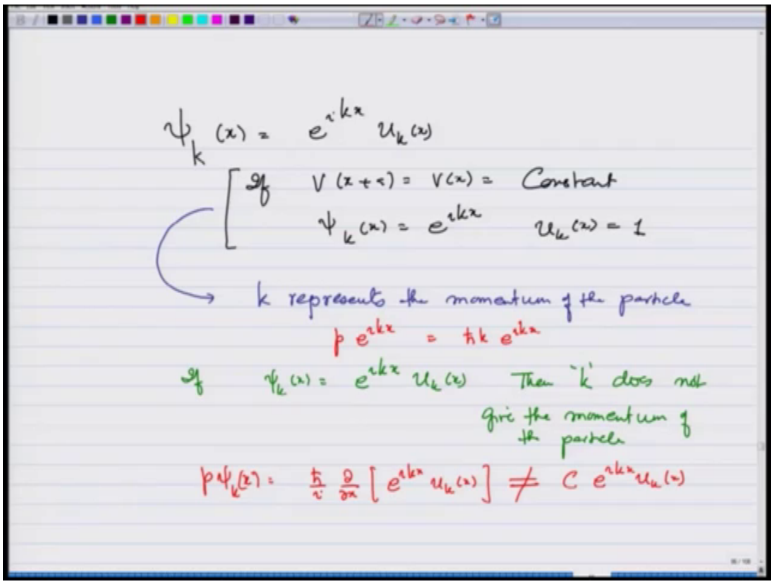

Now, in the wave function I am labelling it by k x is e raise to i k x u k x, right if v x plus a equals v x is equal to a constant. Then I know in that case particle is free and the wave function psi k x is e raise to i k x and u k x therefore, in that case is 1. So, as the potential is increases becomes non-constant, but remains periodic you get this u k which is different from that constant or 1.

In the second case k represents the momentum of the particle, how so; because if I take p operator operating on e raise to i k x I get h cross k e raise to i k x. So, this is a momentum I can state as we have said again and again while discussing these things. Earlier on the other hand if psi k x equals e raise to i k x u k x, then k does not gave the momentum of the particle, because this is not an Eigen state of the momentum.

So, there is the momentum is not conserved. That is also quite easy to see if I do p psi k x this is equal to h cross over I d by d x of e raise to i k x u k x. And this is certainly not equal to sum constant times e raise to i k x u k x. This is not equal to that. So, there is no conservation of momentum. So, momentum cannot really be defined for these states none the less k is a good quantum number which is related to the cemetery that if you translate the whole system by the period a nothing changes.

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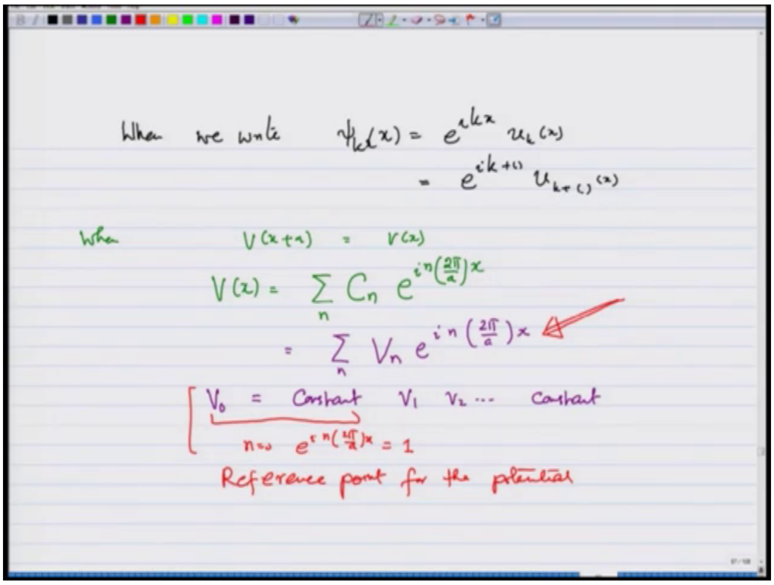

Now, when I write psi k x as e raise to i k x u k x, this can also be written as e raise to i k plus some quantity related to the periodicity and u k plus some quantity related to the periodicity times x, which I am going to explain now.

So, when v x plus a is equal to v x v x can be written in the form using Fourier series, summation of n some constant c n times e raise to I 2 pi over a x times n. And these c ns I am going to call the nth component of v. So, I am going to write this as summation n v n e raise to i n 2 pi over a x. V 0 is basically a constant, and v n v 1 v 2, all these are constants. Now v 0 has a particular significance because n equals 0 gives me e raise to i and 2 pi over a x to be equal to 1. And therefore, what v 0 represents is just a reference point for the potential.

So, it does not really affect the solution all is does is changes a reference point for the energy.

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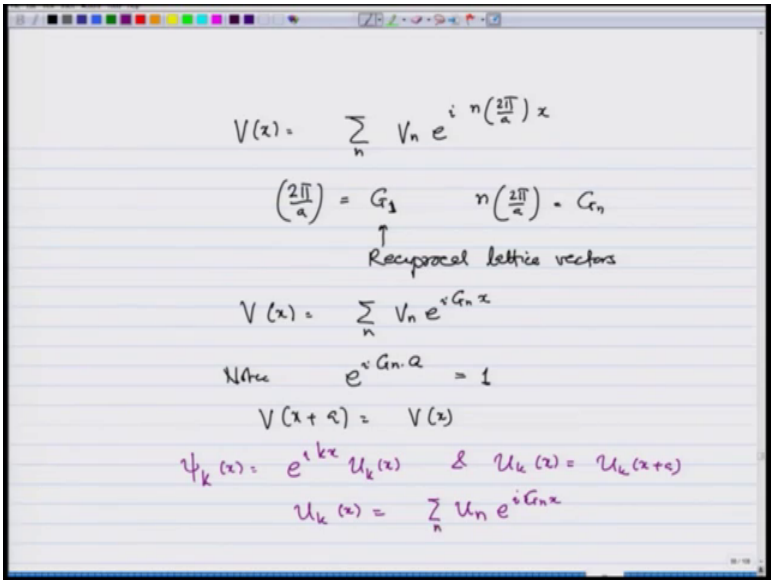

So, the potential components that affect the solution are the components v 1 v 2 and so on. So, we have v x equals summation n v n e raise to i n 2 pi over a x. I am going to call 2 pi over a is equal to G 1 and n times 2 pi over a as G n. And these are called as reciprocal lattice vectors, but that just name I am giving you, but right now let just then therefore, write v x equals summation n v n e raise to i G n x. Notice that e raise to i G n times a is equal to 1. That is by you know Fourier theorem therefore, v x plus a becomes same as v x. So, G n is 2 pi over a and thus reciprocal space or reciprocal lattice vectors

Since psi k x is equal to e raise to i k x u k x and u k x is also periodic. I can write u k x also as equal to sum u n e raise to i G n x summation over n.

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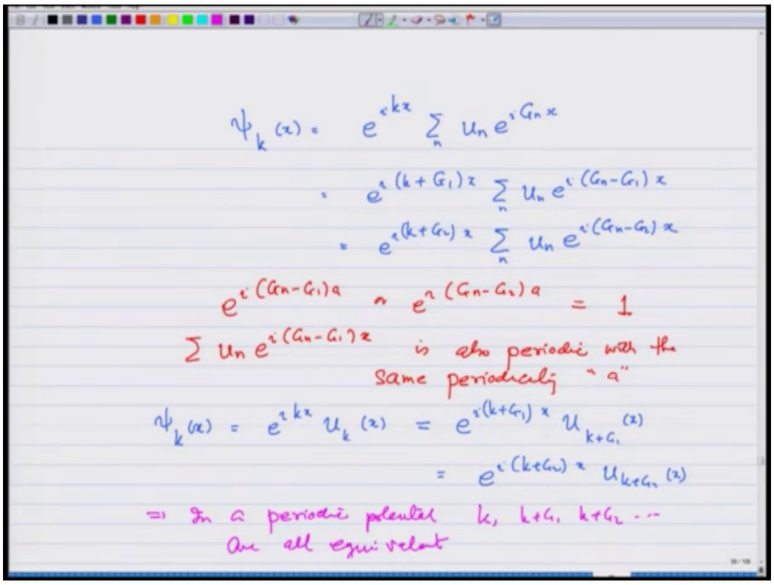

So, I have psi k x equals e raise to i k x summation over n u n e raise to i G n x. I could also write this as equal to e raise to i k plus some specific G let me call it G 1, x summation n u n e raise to i G n minus G 1 x. I could also write this as e raise to i k plus G 2 x summation over n u n e raise to i G n minus G 2 x. Even if I do so, notice that any e raise to i G n minus G 1 a or e raise to i G n minus G 2 a is 1. And therefore, summation u n e raise to i G n minus G 1 x is also periodic with the same periodicity a.

So, I could write psi k x which is e raise to i k x u k x also as e raise to i k plus G 1 x u I will call the function with G 1 as u k plus G 1 x, it is the same satisfies the Bloch's theorem. I could also write this as e raise to i k plus G 2 x u k plus G 2 x. And therefore, the final solution remains the same and therefore, what we conclude is that in a periodic potential k, k plus G 1 k plus G 2 and so on are all equivalent. So, I could label the wave function by either k k plus G 1 k plus G 2 and then we follow a convention that we restrict k 2 within certain boundaries.

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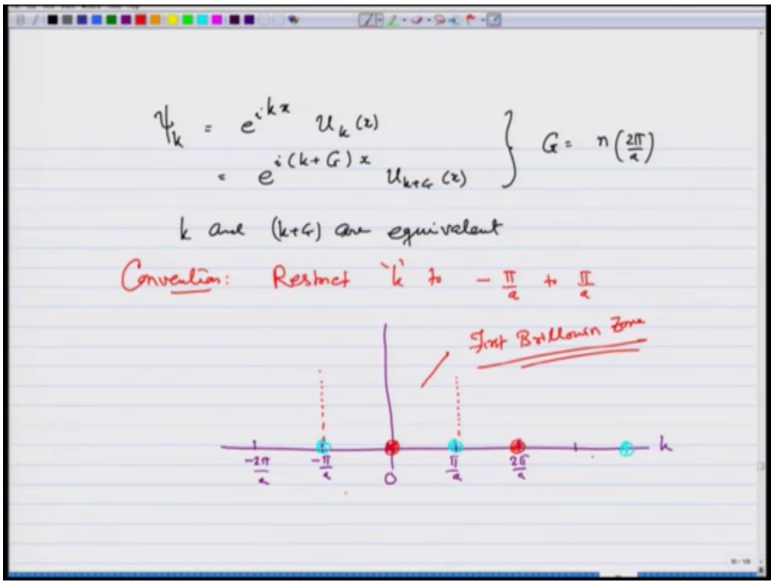

So, what we just seen is that if I have a psi k which is written as e raise to i k x u k x. I could have written this also has e u raise to i k plus some general reciprocal space, vector u k plus G x. And both satisfy the Bloch's theorem G obviously, as I we have been saying is some n times 2 pi over a. So, k and any k plus G are equivalent as far as the wave function is concerned. And this is because the periodicity of the wave function and periodicity of the lattice.

So, what the convention we fallow is restrict k to minus pi by a to plus pi by a. So, just to show it pictorially, if I have k equals 0 pi by a 2 pi by a and so on, minus pi by a minus 2 pi by a. Then what we have discussed So far is this point at 0 which I am showing by red circle is equivalent to this point. Point at pi by a is equivalent to minus pi by a and so on. And this 2 by a is equivalent to then 4 pi by a and so on. So, what we do is instead of specifying k over all these we restrict our k to within this minus pi by 2 pi by a and therefore, then we actually map the entire k space.

So, this is known as the first Brillouin zone. So, we work within the first Brillouin zone, I am just giving you these words. So, that if you hear them you do not really feel intimidated what it is all these are equivalent. So, I can restrict myself to working within k within minus pi by a to pi by a.

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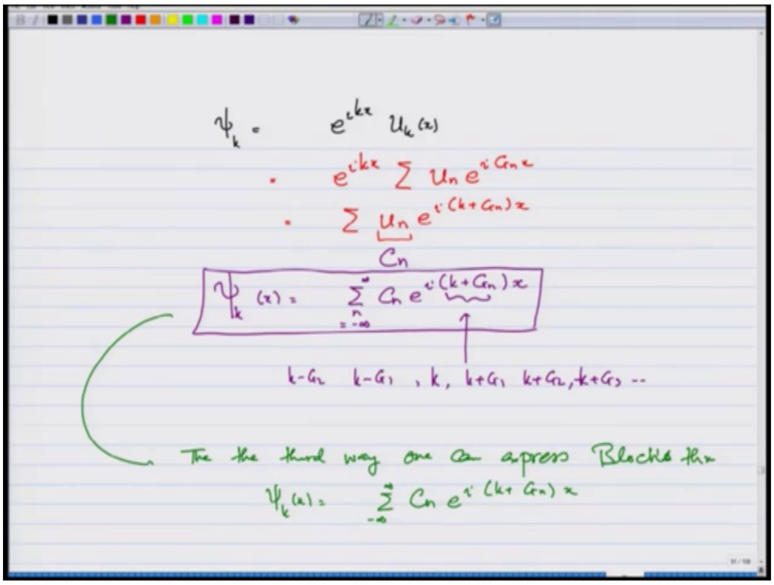

Now, write the solution because we wrote psi k equals e raise to i k x u k x. And since u k is periodic we wrote this as e raise to i k x summation u n e raise to i G n x which I can write as summation u n e raise to i k plus G n x. Just for the convention sake let me write this u n as c n some coefficient c n.

So, I am writing my psi k x equals summation n c n e raise to i k plus G n x. This is another way I can write the wave function. And you see this wave function carries all momenta k, k plus G 1 k plus G 2 k plus G 3 and so on. K minus G 1 k minus G 2 and so on, and varies from minus infinity to plus infinity. And therefore, it does not really matter whether I specify the wave function by k k plus G 1 k plus G 2 k plus G 3 it is another way of seeing that all these are equivalent if they are all equivalent again I will restrict myself to k being between minus G 1 by 2 to G 1 by 2 in the first Brillouin zone.

Now, once we have this equation. So, this is the third way, one can express Bloch's theorem. That is that psi k x is of the form summation minus infinity to infinity c n e raise to i k plus G n x. And this form is useful in writing the equation for the c ns and then from that getting the band structure. That is why introduce this.

So, I will just conclude this introduction to Bloch's theorem.

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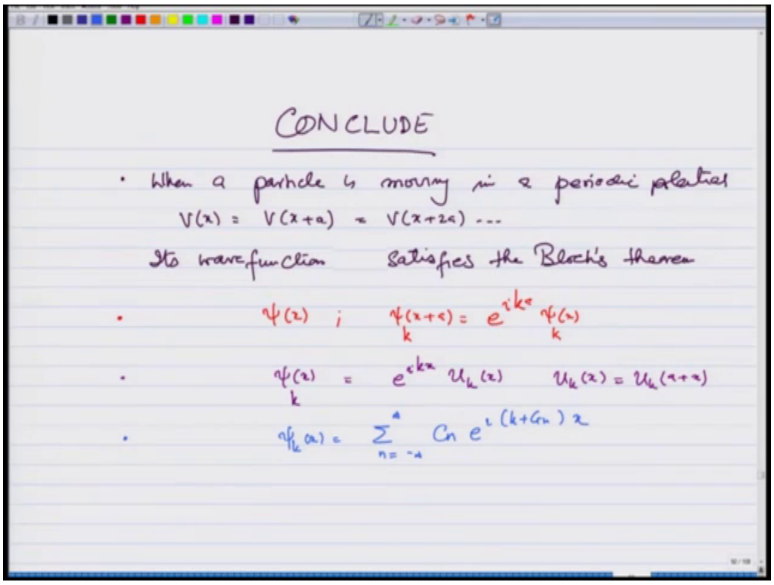

So, conclusion when a particle is moving in a periodic potential, v x equals v x plus a is equal to v x plus 2 a and so on, it is wave function satisfies the Bloch's theorem. What is Bloch's theorem? So, psi x is such that psi x plus a is equal to e raise to i k a psi x, and we label this by k. This can be expressed in another form that psi x again I label it as k is equal to e raise to i k x u k x where u is also periodic u k a plus x.

And finally, I can also write this as psi k x equals summation n equals minus infinity to infinity, c n e raise to i k plus G n x.