Physics of Materials

Prof. Dr. Prathap Haridoss
Department of Metallurgical and Materials Engineering
Indian Institute of Technology, Madras

Lecture No. # 33

Calculating Allowed Energy Bands and Forbidden Band Gaps

Hello, welcome to our 33 rd class in the Physics of Materials course that we have been going through and we will continue from where we left of last class. When I finished last class; I told you that, what we had done was to pictorially see, how bands of energy, allowed bands of the energy and band gaps appear in materials, as a result of the interaction of the wave vectors corresponding to the nearly free electrons and periodic structure of the lattice.

So, we had seen it periodic in in a pictorial sense, we actually drew the periodic structure, we drew it all the same scale in k space, we drew the reciprocal lattice in k space, we looked at the allowed wave vectors in k space and we found that when you plotted both the information at in k space, we could identify the locations where the the parabola corresponding to the electron energies intersected the boundaries of those Brillouin zone right.

And at those points of intersection the, we set in term in a descriptive sense, there are that point the k vector corresponding to those energies, satisfies the condition for diffraction. As a result of diffraction, there is the distortion of the e versus k relationship in region very close to the Brillouin zone boundaries, the result of this distortion is that we have specific values of energy that are now prohibited.

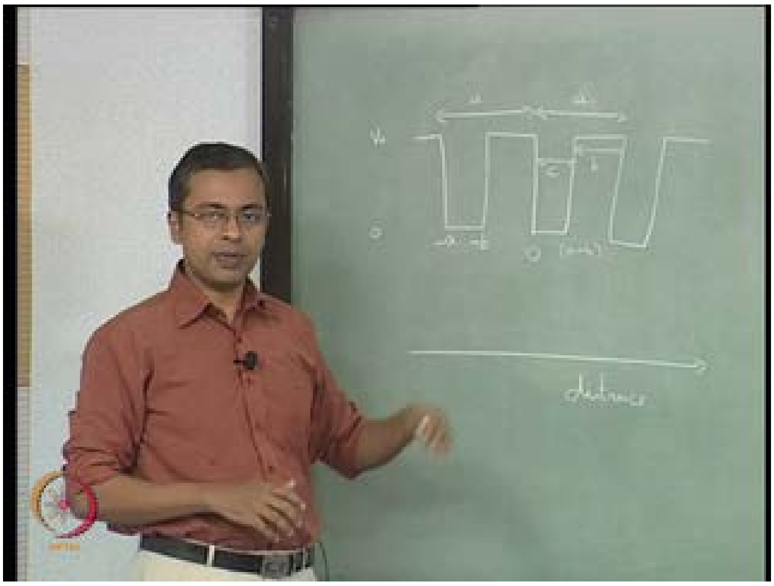
So, as a result we were able to see, how allowed energy levels and band gaps originate in a material all right. So, this is fairly important understanding that we have now got of the material in terms of something fundamental in the material. And we were also we also incorporated in to this picture at the fermi energy level, and that then tells us that given this band structure that is possible in the material and given the fermi energy level that exist in the material, is it just going to be a metal, is it going to be a an semi conductor or an insulator.

So, all of that information we were able to put together, we saw it in a very detail manner for the one dimensional solid, and then we also saw pictorially how the same information would begin to appear for a two dimensional solid, and briefly we saw also for a three dimensional solid, how the fermi surface interacts with the Brillouin zone. So, in this process, we were able to see how, lot of the information we have learned over the last several classes, lot of the terms we have learned over the last several classes, how all of them come together and give us very good understanding of what is happening in a material, and how we described.

So, in the present class we, what we are going to do is, now that we understand that the interaction of this k vectors and the Brillouin zone leads to, and this is periodic structure leads to this energy gaps that appear.

We will go through a calculation, we will see if we can actually calculate when we are going to have an allowed energy level, and when we are not going to have an allowed energy level. So, it is this calculation that we will go through in this class, and in this process, you will see what sort of in an approach we can take to put numbers it down to this problem. So, to do that, we will start with a brief look at what is the system that we are going to evaluate, and then we will go about a writing the equations down for the system and evaluating the system.

(Refer Slide Time: 03:37)



So, basically we have going to have a series of potential wells. So, I am just drawing three potential wells here and we will mark this as the origin of this diagram and this is the distance. And we will say that the periodicity of this structure is a, so when we say periodicity, so we are basically saying if you start from here ah., we come down, we go through this structure here, and then again come out here. So, we have to comeback to the same location. So, that could be the periodicity of the structure, we will say that the width of the potential wells is c, this distance between these potential wells is b, right and the periodicity of the structure is then a.

So, we can you know designate periodicity as a here, which means from here to here is what it would be, it will come back to the same location. So, this would be the a that we are looking at, or if you are looking at from here, this could be the a. So, this is this is a or this is a, where we are coming from the same location to the same location. Therefore, this is a, this is the periodicity of the structure a. So, if you write this as the origin, this is basically minus b, and this is minus a location, and this is then a minus b, this is also a (Refer Slide Time: 4:58).

So, this is the periodicity of the structure and all the details are now available here, we will say that you know that potential here is 0 is basically 0, and this is some v 0 potential that is there. So, in other words, there are regions where the potential drops to 0 which is the potential well that we have, and then there are regions where the potential is the v. So, this is the V naught, so and these are all relative number. So, it does not really matter, because we are going to look at relative potentials with respect to some scale. So, this is what we have, and we would like to see what is occurring in the system, what is allowed in the system, what is not allowed in the system and so on.

So, to do this basically, we are looking at the bunch of electrons which which are now subject to this condition, the conditions that are shown here; with respect to this, so we have to see, what is the impact of the conditions on these conditions on those electrons, we have to basically solve the Schrodinger wave equation for the electron subject to these conditions. So, it has some energy e and it has, it is faced with the potential v naught in some location, it is faced to the potential 0 and some location.

bSo, with respect to that we we it solve the Schrodinger wave equation, basically we see that you know we have some specific boundaries where you can solve the Schrodinger wave equation of this side of the boundary; where the potential is v naught as well as solve the Schrodinger wave equation on this side of the boundary where the potential is 0.

So, these are two possibilities that we have, what we are going to do is, we are actually going to do that way, we are going to solve the Schrodinger wave equation where v equals v naught and we are going to solve the Schrodinger wave equation where v equal 0, and they are going to required that at the boundary, these two solutions are give us the same volume. So, this is based on our general understanding that such functions have to be reasonable, the solutions that we get have to be reasonable which implies that, we are going to say that it is going to be continuous.

So, in terms of the value here and in terms of the slope here, the function on a either side of this boundary, whether it is coming from the v v naught side or it is, whether it is coming from the 0, v equal to 0 side, the value should work out to be the same and the the slope of those functions, or the derivative of those function should work out to be the same.

So, that will then give us two equations for this system, there is another, so that is how we would get two equations, and we will find there are certain constants that we need to figure out.

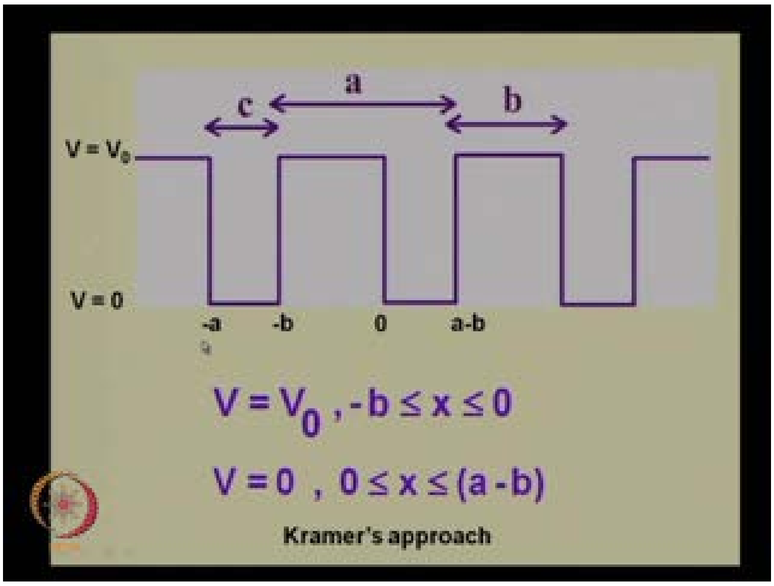
Additionally, we have periodicity in this lattice and there is the way to represent periodicity in in terms of the wave function, and that periodicity will ensure that we can compare two other locations in this system which which are then periodic and then for those two locations, we can again again say that you know for those two locations, we have to have the value of the function to be the same at the two locations and the derivative to be same. So, in this process for two different locations, we are going to get based on these two analysis that we have just described, we are going to get four equations.

We will find that there are four constants in those equations, which we can attempt to solve for, what we will see is, our end goal is not to really solve for this constants. But this provides us the framework, we will go ahead an attempt to solve for those four constants, but we will not worry about the actual solution of the four constants, will find that end root we will reach, we will we will reach an expression, we will reach an equation which will now have certain values which are correct and certain values which are observed.

So, the range of values over which were getting the, where the equation is meaningful will then become allowed, will represent then the energy, allowed energy band and range of values where the equation is no longer meaningful will then become the band gap. So, that is how we will see that you know this set of constraints, and what we are solving with respect to be constraints gives us when we are going to have a allowed energy level and and when we are going to have a band gap, this is what we are facing and that is what we will see.

So, we will set it up as we are going to solve for all the constants, but actually we will not bather to solve for the constants, we will just used this as the frame work to get us what we need. So, now we will look at a series of slides which we will start with the diagram like this and then it will solve a set of the equations which will get us the result that we are interested in.

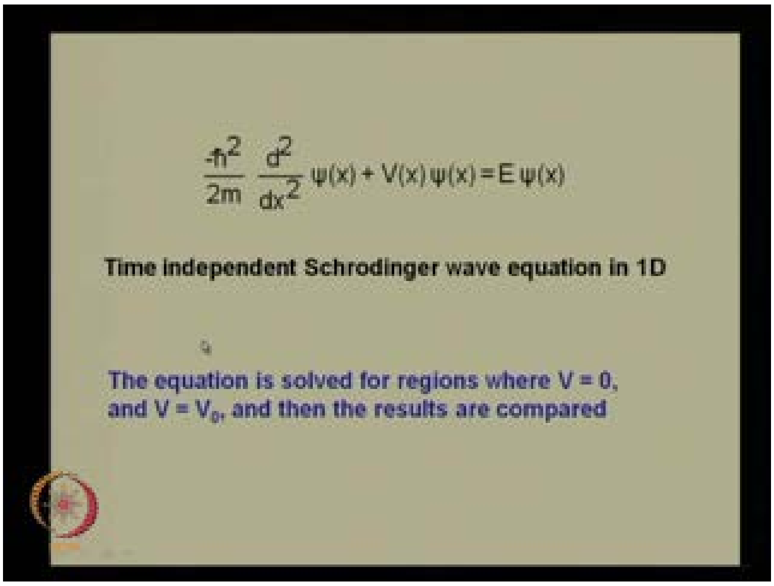
(Refer Slide Time: 09:27)



So, this is the system which we have just drawn. I just showing you again here, this is the width of the potential well that we have, and this is the periodicity of this structure that is sh0wingup here, and then we have the distance between the potential wells. And again as we had just drawn, this is we, arbitrary designate this as the origin. And therefore, this would be minus b that is the width backwards, and then this is minus a, and then this location would be a minus b; if you just did it, you will get it.

And to put it down in numbers, V equals V 0 which is this value in the region minus b to 0. So, from here to here, minus b to 0, V is equal to V 0, so that is what is written here. And similarly, V is equal to 0 for 0 to x b, when x is between 0 and a minus b which is this region right, between 0 and a minus b, the potential is 0, and this general approach that we are showing here is attributed framework. So, that is what we are going to see.

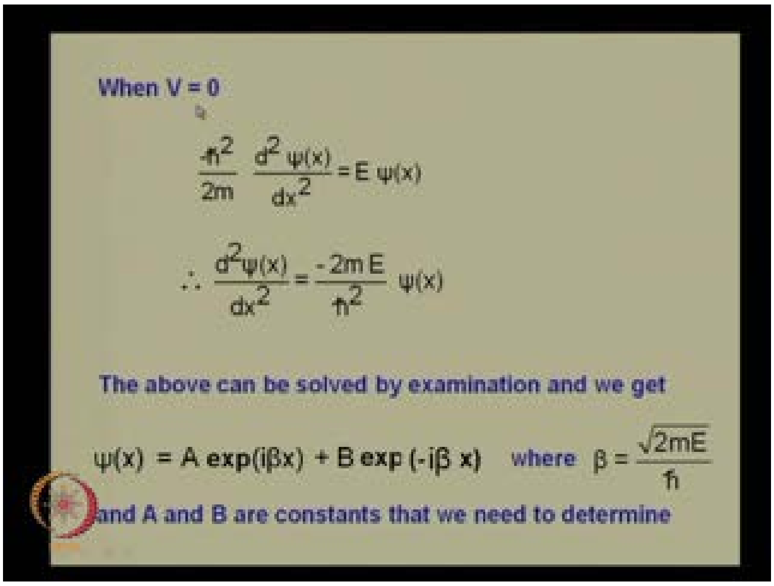
(Refer Slide Time: 10:30)



So, what we have to do is, we have to solve the Schrodinger wave equation. In this case, it is the one dimensional system we are looking at. So, the time independent Schrodinger wave equation which we looked at in one of our earlier classes is what is represented here, in this essentially it says that the total energy is equal to the potential energy plus the kinetic energy, so that is basically what is what it says.

We have to solve this equation for conditions where the potential is 0, and for conditions where the potential is V 0 as supposed 0. And we will say that, when we compare these results in terms of the derivatives, in terms of the actual value of the the wave function as well as the derivatives of the wave function, based on the comparison, we will be able to find out the solve and get us get us the result that we are interested.

(Refer Slide Time: 11:23)

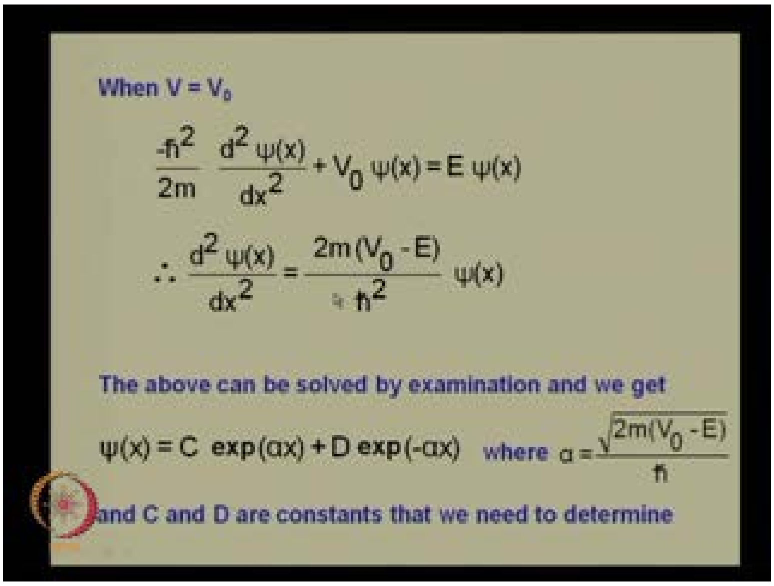


So, when V is equal to 0, if you go back here, this term become 0. So, essentially this term has to equal this term here, so this term will go away. So, that is basically what you see here, h bar square by 2 m, minus h bar square by 2 m d square psi by d x square equals E times psi. So, if you rearrange it, you have a second derivative of the wave function d square psi by d x square is minus 2 m E by h bar square by psi x, this can straight away be solved by examination, merely by examination.

Because you know any exponential function, if you differentiate it, you will sort of get this; if you differentiated it twice you get this plus you have a negative value here. So, that is why we need to look settled it up this way. So, psi x of the form A exponent minus exponent i beta x plus B exponent minus i beta x will solve this equation.

So, if you just derive it, differentiate twice, you will get the beta square showing up out here and the beta square times psi x is what you will get, and the beta square is this value here, therefore beta is simply the square root of it, of this 2 m E by h bar square. So, beta it is what you have here and the i takes care of this minus sign. And A and B are constants, that we do not know what they are at this point, and we will the need to determine. So, this is how this equation works out and similarly, we can attempt to solve the time independent Schrodinger wave equation, in under the conditions where V of x is actually V 0. So, it is some finite value V 0 which as not 0.

(Refer Slide Time: 13:01)



So, to do that we have to go here, we just rewrite the equation. So, again it is h bar square by 2 m minus h bar square by 2 2 m d square psi by d x square plus V naught psi is the E psi. So, rearranging you get this 2 m by V naught E by V naught minus E by h bar square psi x, simply I have just taken this values and move this to this side, and then rearrange again this can the solved by the examination except that we will now get.

We get function that look like this, C exponent alpha x plus D exponent minus alpha x. Please note that when we previously solved when V is equal to 0, we got solution like this, now E power i theta equals cos theta plus i sin theta. So, these are actually trigonometric functions which will which will essentially be sinusoidal functions.

So, this solution is a sinusoidal solution, and that results because you have this i here which comes again because you have a minus sign here right. So, that is how these things are tied together. If you look at our new solution now in the presence of a potential V naught, the term alpha which is similar to the term beta we had in the previous equation, it has this form, root of 2 m V naught minus E by h bar.

Now, clearly this value any here can be negative if V naught is less than E, and it is positive if V naught is greater than E. So, if when V naught is less than E, or rather the energies of the electrons are higher than the V naught, then actually this works out to be a negative value in which case it is it is a same as saying to have a i out here.

So, therefore, so the square root of minus 1 will once again appear. So, when the energy is greater than V naught under conditions where energy is greater than V naught, this solution will also be sinusoidal, just the way the previous solution was, because there is a square root of minus 1 is going up in both these terms. On the other hand, when V naught is greater than E or in other words, the energy is less than the value of V naught, energy of the electrons the less than the potential that it is facing.

Potential V naught spacing, this will remain a positive value in which case these are all, the alpha remains the positive value and real value. And therefore, these this equation translates to an exponential equation. So, again we have two constants here, C and D which we need to determined. Now, let us before we proceed further, let us look carefully at what we have got here.

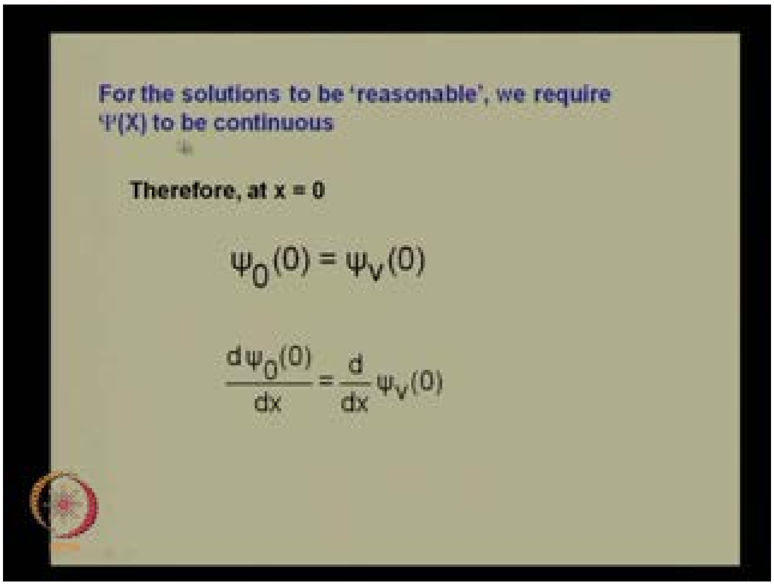
So, x is the location so x is the location, so that is along the axis. So, that is something that we can vary, now alpha that we have here and also that we have here consist of this information here, it is 2 root of 2 m, so m is the mass of the electron. So, that is fixed, h bar is fixed, the V naught that is there for that system is also fixed. And this energy is something that we are not yet sure of it, it could be arrange of energy, we will have to look at the solution for a variety of energies, so this is what we have.

In other words, the alpha actually has many of the system details and it, the V naught is from the system and h bar is from the system. Therefore, it contains the lot of system details, so it is not something that we have lot of I mean there are too many things that are unknown out here, except we will try out from range of energies here, C and D we have no idea what they are at this point, we have to find out what they are.

Similarly, if you go back to the previous solution that we had, again we see the same thing, the beta that we found there also has 2 m here, m is again something that is fixed, we do not have a choice of h bar is fixed. So, it is for a range of energies that we are going to check it so that we will have different values of beta, but it is something that again system based.

So, it is only A and B that we do not know how to here, which we have a absolutely no idea what they are, x and again is the dimension or the direction in distance that we are, or position that we are checking this function. So, we now have this solution, we have solved this, we have the general form of the solution for psi of x both under conditions where B is 0 as potential and V is V 0 as potential. And as I mentioned our intention is to actually compare these solutions, add specific values at convenient locations, and see what that convenient location helps us understand about the system.

(Refer Slide Time: 17:20)

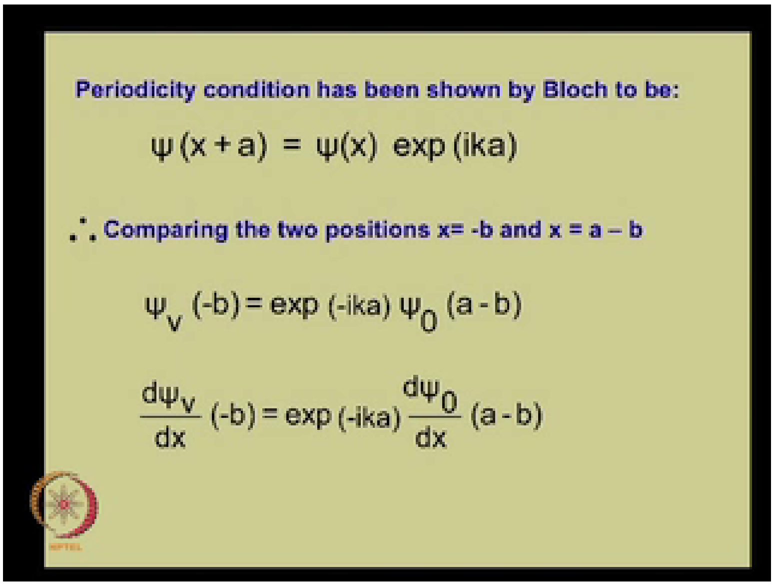


So, as I said for the solution to be reasonable, we require that psi of x be continuous, therefore at x is equal to 0, at that location x is equal to 0, we we would like the function, the wave function of that at x is equal to 0 to be the same regardless of which direction you are approaching that 0 from. As we saw in our original in the first slide, we can approach it from from the direction where the potential is 0. So, that is why the subscript 0 is, or we can approach from the direction of the potential is V, in fact V naught, but we try to have be here.

So, we can approach, so we can have a value for psi at the position 0 when approached from the direction was potential is 0 and we can have a value for psi when position is 0, but when we are approaching it using the solution from the direction where V is the potential and we also required that the first derivative the the same.

So, same thing we can differentiate the solution coming from the direction where the potential is 0. In other words, we differentiate the solution that we got when the potential was 0 and we will differentiate the solution that we got to the potential was V, we will substitute 0 in both those solution and equate them. So, we are saying the this is going to be required of the system for the solution to be reasonable, similarly we will also do this once we find out what the affect of the periodicity of the lattice is, and we will incorporate the same thing with the periodicity, the value of the function was going to be the same in to different locations and the value of the derivative is going to be the same two different location.

(Refer Slide Time: 18:50)

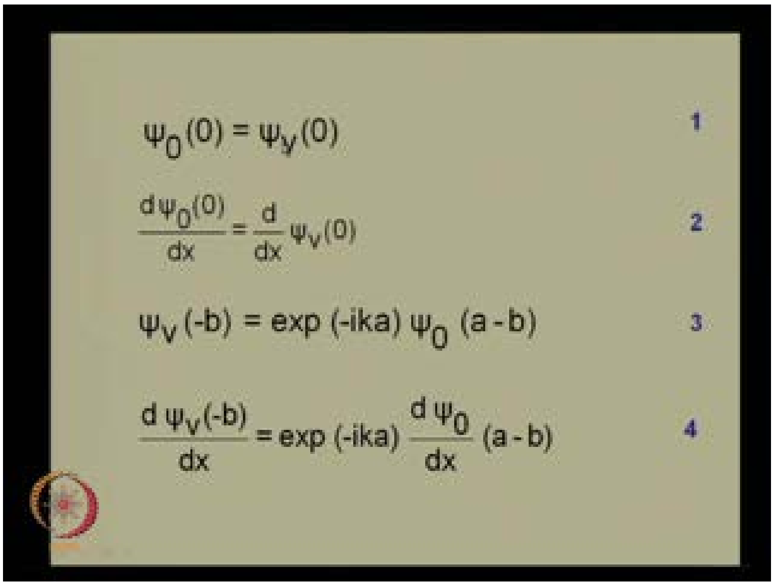


So, the periodicity, of a periodicity condition and such circumstances has been shown by block, person block, he is credited with this. So, he basically says that you know in terms of the potential, we say essentially v of x plus a is is the same as v of x when a is the periodicity of that structure. In this case we are saying that, wave function x plus a psi of x plus a will be the wave function at psi times exponent minus k a where k as the wave vector and this takes into account the periodicity at the interaction of the periodicity with the wave vector.

So, that is how this comes about and that is the reason why we have this additional function. So, if you put it in that is how we will get it. So, if you put in x plus a and you expanded, you should get this psi x exponent i k a is that coming out of the equation. So, that is how this periodicity comes about. So, therefore, now we can locate two positions which are not originally in the previous light, we actually looked at x is equal to 0, so therefore, at that point we looked at the solution from the same location.

So, to speak, so we were not really looking at two different locations, we were looking at the same location. Now, we are actually looking at two different locations, we are going to look at location which is x is equal to minus b and another location where x is equal to a minus b, they are comparable because of periodicity.

(Refer Slide Time: 20:13)



So, psi 0 is what we have here, so on both side it has to be same. And the differential of it at, when you differentiate the equation on of the wave function on either side of the origin, the different the slopes should workout to be the same. So, that this is the, what we discussed. So, based on the solution we have got for a psi 0, we can actually once you incorporate x is equal to 0 at the solution, we will get one equation. Similarly, once you differentiate it and you put x is equal to 0, you will get another solution, our another equation.

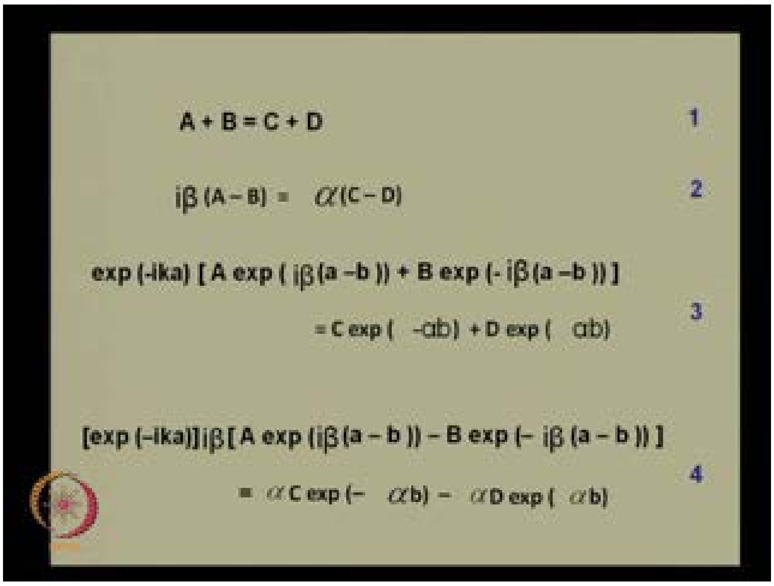
And then similarly, you can take the value of psi at the potential V at this location minus b, and if you equate, if you workout this expression, then the equation that you will get will be equation 3. And similarly, again you differentiate this equation on both sides, you are and you are requiring that the slope be the same, therefore you will get a equation 4.

So, therefore, looking at two locations, one is at though origin. So, the all of these two equation look at the origin, they are basically saying that the value of the wave function on either side of the origin should be the same, the slope of the wave function on either side of the origin should be the same, that is basically all it says, and the one one side of the origin we have a potential 0; on the other side of the origin, we have potential 0.

So, that is what these two equations say, so simply using the solutions, if you do this equations, we will come up with two equation corresponding to these two. Similarly, we what we are saying here, based on periodicity, the value of the wave function on one side at the particular location should be this term times the value of the wave function on at a at a other location. Again coming from one side which is potentially equal to 0, it to another side were potential is V, at the same thing this slopes on either side with this factor (( )) should be, workout to be the same.

So, this is how we have got these four equations and they directly relate to the system that we have just described.

(Refer Slide Time: 22:07)



So, if you go in here, if you just evaluate these four equations that I have put down here, for all these four equations I am simply taking the solution at psi is at v equal to 0 and the solution at v equal to v naught and then working out these the left hand side to the right hand side of each equation. So, for example, if you look at this first equation, so we are simply saying that the solution on the side that is where the potential is 0 is equal to the solution where is on the side where the potential is v at the point 0.

So, if you go back to what we just solved, we see that when potential is 0, so we have this solution. In this solution, when you incorporate x is equal to 0, this terms works out to 0, this term work out 0, therefore this exponents workout to one (Refer Slide Time: 22:50).

So, simply psi of x works out the A plus B all right, so psi of x at x is equal to 0 and the potential b equal to 0 is simply A plus B. If you go to the next equation on the the right hand side was the psi of x when the potential is B, and and the (( )) position x is equal to 0 when potential is v, this is the solution and when x is equal to 0, this is again 0 and this is again 0 (Refer Slide Time: 23:17).

So, these two terms to work out to 1, therefore this become C plus D. So, therefore, as saying that the psi of when you put this equation down here, when we say that psi of 0 at the point 0 is equal to psi of v at the point 0, this simply means A plus B, this is this is works out to A plus B, this work out to C plus D. So, that is what we have, the first equation gives us A plus B A plus B is equal to C plus D.

Similarly, if you go it go back to those same equations and differentiate then, so which we just do briefly, if you differentiate this with respect to x, you will get a factor i beta out here. So, it this will become i beta A, exponent this parameter here, and if you differentiate this term you will get minus i beta B, exponent this parameter here, one second when you substitute x is equal to 0, the exponential parts in drop to 1, (( )) both of them will drop to 1.

So, therefore, we will have i beta A and minus i beta B, if you take this equation where v is equal to v (()) and differentiate it once, you will get alpha C exponent alpha x minus alpha D exponent minus alpha x. And then if you put x is equal to 0, this will become 1, this term will also become 1, so therefore this is simply be alpha C minus alpha D. So, if you go go back here, so we are going to have on this side alpha C minus alpha D and this side we are going to have i beta a minus i side beta b.

So, that is how this equation will give us this equation that we see here right. So, you now understand how we are getting this equations, these two equations here look a little bit more complicated, but they are actually not, they are exactly the same procedure that we have followed for these two equations, except that we are we are actually using this bottom two equations.

So, you see where this exponent minus i k a term comes here so that you will see here in all the spaces, exponent minus k a will show up here, minus exponent minus k a it shows as here right. So, that term shows up in both spaces and we are just evaluating this function psi V at of position minus b and we are also evaluating it is derivative at the same position minus b.

And similarly, we are evaluating psi 0 at the position a minus b and its derivative at a minus b. Previously, if these these were 0 and therefore, we we were able to remove the several terms, but now they have some specific values, because you have a minus b.

So, the simply if you just do that, you will get the expression that you see here. So, the value of the periodicity condition will give us this expression that, we this equation that we see here, and then when you differentiated and you write, again incorporate the periodicity condition and then differentiate it and expect the derivatives to be same on either side, then you get this equation here all right.

So, we now have four equations, 1, 2, 3 and 4, four equations quite straight forwardly we can associate them with the wave equation, how be solved at based on the wave equation, I suggest a that give you go ahead in a do this on you on just so that you see how this they come about. But the procedure I have shown you is exactly with procedure, you have to follow you nearly have to go through the numbers and you will find that this is what you get.

So, this is the, these are the two equations the four equations that you get. Now, in these four equations, I will again (()) that A, B, C and D are the constants that we have, no idea what they are, alpha and beta, alpha here and beta here contains system related details such as the depth of the the potential well and such. So, that is what it contains in the mass of the electron. So, that is what is contained here, and k is the wave vector.

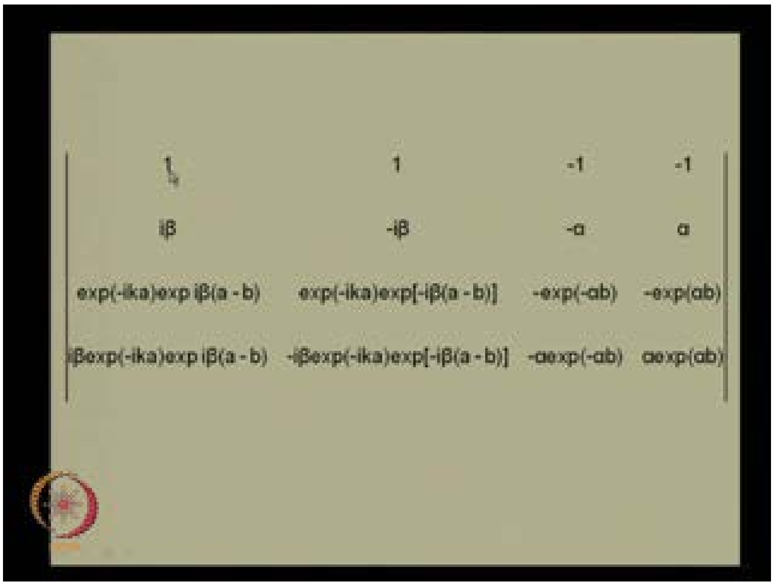
So, that is what is here, everything else is the simply a mathematical term here. So, to speak, so this is what we have here and what we can do now is, in fact now that we have four equations where we have four unknowns A, B, C and D. It allows us to use mathematical approaches to try and solve for A, B, C and D.

However, I will point out that we have the mathematical approach, we will take is to attempt the solve for A, B, C and D, but that is not really our end goal, our n goal is nearly to actually see what are the conditions under which energy, we have permitted values of energy and what are the condition under which we have forbidden values of energy. So, this is simply a framework to help us get that information.

So, we will we will proceed to try and solve for A, B, C and D and at some point you will actually abandoned that attempt and we will we will use an equation that comes up in the process, because that itself is what is the information we are looking for. So, to solve this first of all we just we merely have to write this as A plus B minus C minus D equals 0, and similarly move everything to the left hand side, appropriately this set as all to 0 and we have four equations and four unknowns.

So, therefore, to solve this we have the mathematical principle that we required to adopt approach, we need to adopt is that the coefficient of A, B, C and D in this four equations, that determinant of those coefficients should evaluate to 0. So, the determinant of those coefficients should evaluate to 0. So, for example, from the first equation when you write this as A plus B minus C minus D equal 0, the coefficient are plus 1 plus 1 minus 1 and minus 1, because these two will be on the side of the equal to sign. Similarly, you are going to have plus i beta minus i beta minus alpha plus alpha as the four coefficients of A, B, C and D, once you move this term to the LHS and equated to 0 all right. And similarly, you do the same with these two equations and so, we will get the determinant that looks like this.

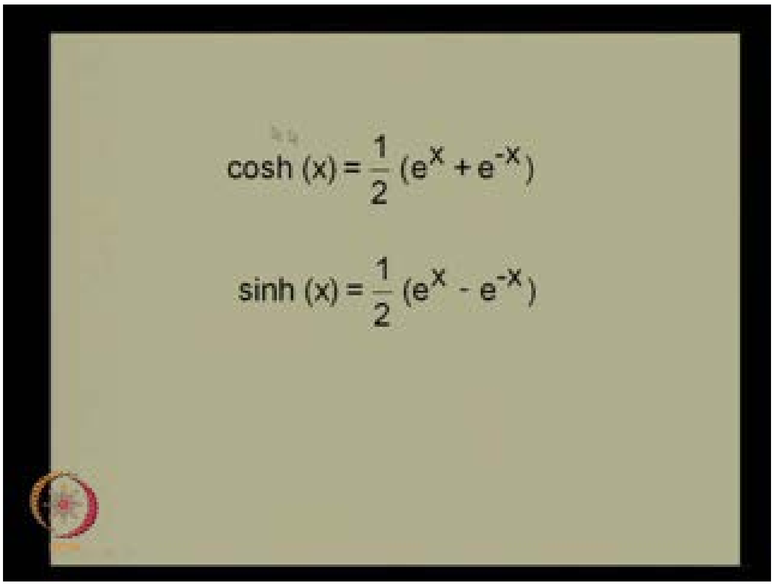
(Refer Slide Time: 28:59)



So, we as a said we have 1, 1, minus 1, and minus 1, we have i beta, minus i beta, minus alpha and alpha. If you look at the other two equations, this is how the coefficient will work out, so the coefficients are all listed here.

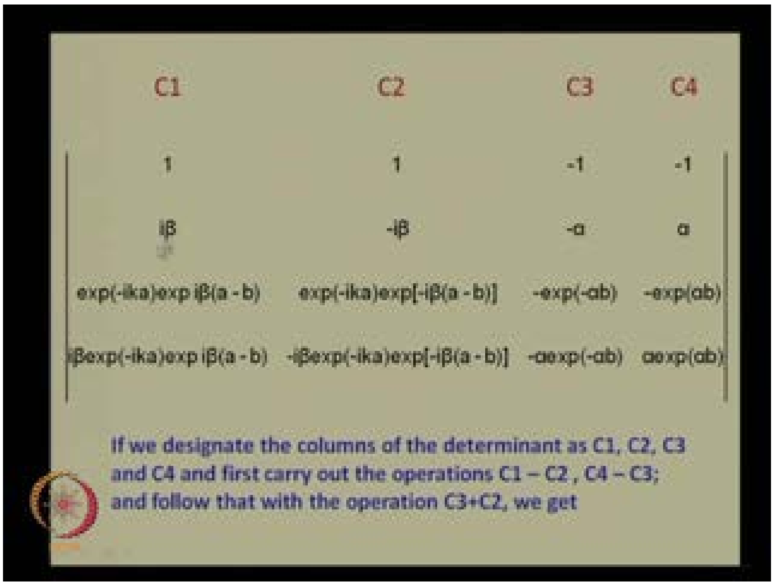
And so, this is the determinant that has to evaluate to 0, when this determinant evaluates to 0, you can use that to solve for A, B, C, and D, so that is how we need to do it. And as as indicated, you can run through this exercise, I am going to show you all the steps involved. So, you can look at these slides and try and solve it yourself, and or you can run through your own solution and then compare it against solution that you see here all right.

(Refer Slide Time: 29:40)



To do this, we are also going to take advantage of this mathematical identities, the cause hyperbolic function of at a of a value of of x is simply half e power x plus e minus x and sin hyperbolic x is half e power x minus e power minus x, these are all standard mathematical functions, hyperbolic functions. And since you see e power x and e power minus x, and we also have them in our equations here, we have exponents some minus x and plus x and so on. So, clearly there is scopes for us to play around with these functions and represent them using hyperbolic function.

(Refer Slide Time: 30:23)

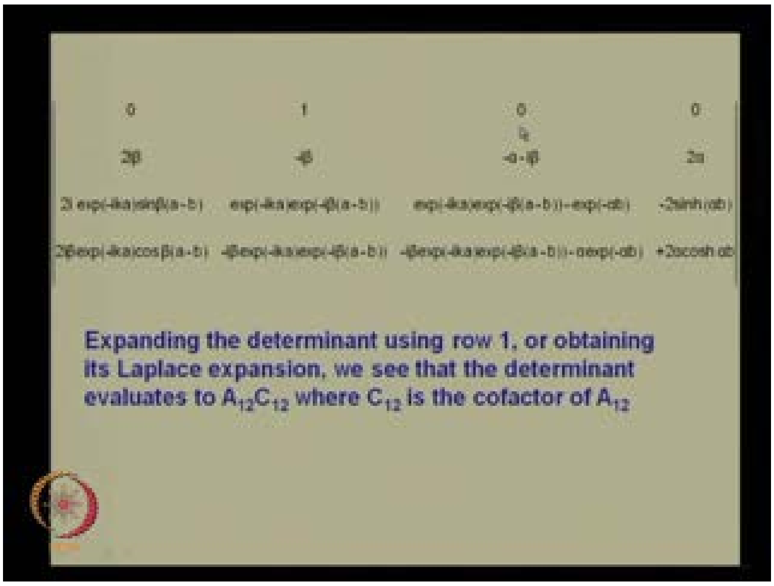


So, that is the reason why we using, so taking advantage of these functions as and when we need them are ah, if will look a determinate again, we have I just rewritten our determinant here, I have not made any changes to determinant and we simply designate them as column 1, column 2, column 3 and column 4. So, I am just walking with through the steps so that you know exactly how we are arriving at our solution.

So, if you designate the columns of that determinant as C 1, C 2, C 3 and C 4 and then let us carry out, see I have purposes to solve the determinant. So, we will simply carry out operations and replace C 1 by C 1 minus C 2. So, if you do C 1 minus C 2 and replace C 1 by C 1 minus C 2, this is going to reduce to 0, because 1 minus 1 will give us 0. And similarly, if you do C 4 minus C 3, so C 4 gets replaced by C 4 minus C 3, so minus 1 minus of minus 1, so that become a 0 again.

And finally, we also do, we replace C 3 by C 3 plus C 2. So, we will add minus 1 plus 1. So, all this are allowed determinant operations. So, you can see that by just doing these operations, we are left with the 1 at and the column C 2, this becomes 0, this becomes 0 and this becomes 0, correspondingly all this terms will also change based on the same additions and subtractions that we are just carried out now (Refer Slide Time 31:24). So, just doing this operations, you will get the determinant we look like this.

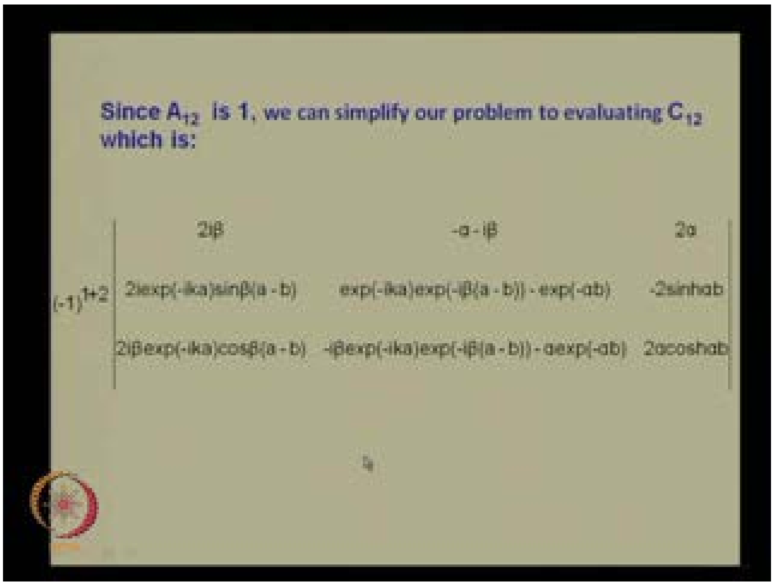
(Refer Slide Time: 31:40)



You have the 0 here, you have 0 here, and you have 0 here, you simply have 1 here. Now, we can expand this determinant using row 1, because three terms are 0.

So, affectively we are we only have expanded using this term, and we can ignore these term. So, we will only we have this, and this, and this, incorporated in this determinant, we can expand that determinant using row 1, or in other words, we can obtain Laplace expansion. We see that the determinant now with evaluate to A 1 2, C 1 2. So, first row second column that is what A 1 2 is, and C 1 2 is the cofactor of this first row second column, which is simply the terms here multiplied by the appropriate factor in the front. So, C 1 2 is the cofactor of A 1 2, so if you do that, so now we are going to simply a expand about this A 1 2 and about row 1.

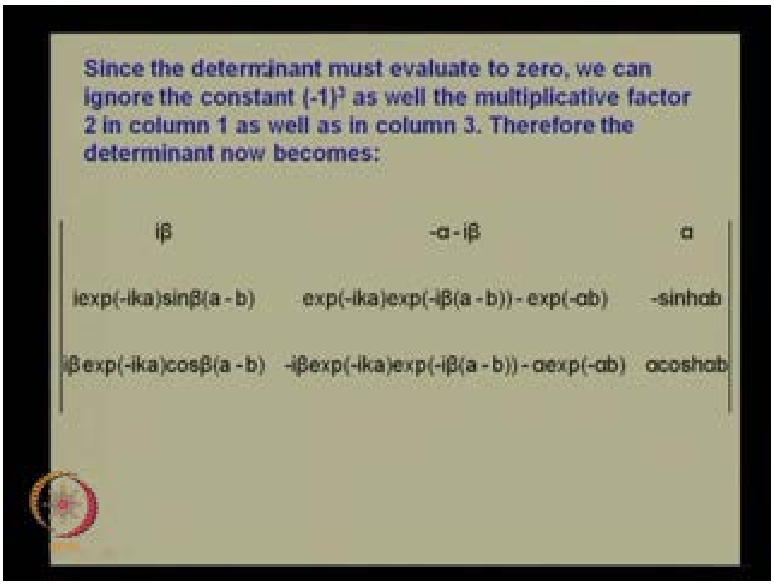
(Refer Slide Time: 32:31)



So, this is what we get, since A 1 2 is 1, we can simplify our problem to simply evaluating the cofactor C 1 2, because A 1 2 is 1. So, we only now have to evaluate C 1 2. So, C 1 2 is simply this, these three terms here, this set of terms here, this set of terms here and this set of terms here times a factor in the front.

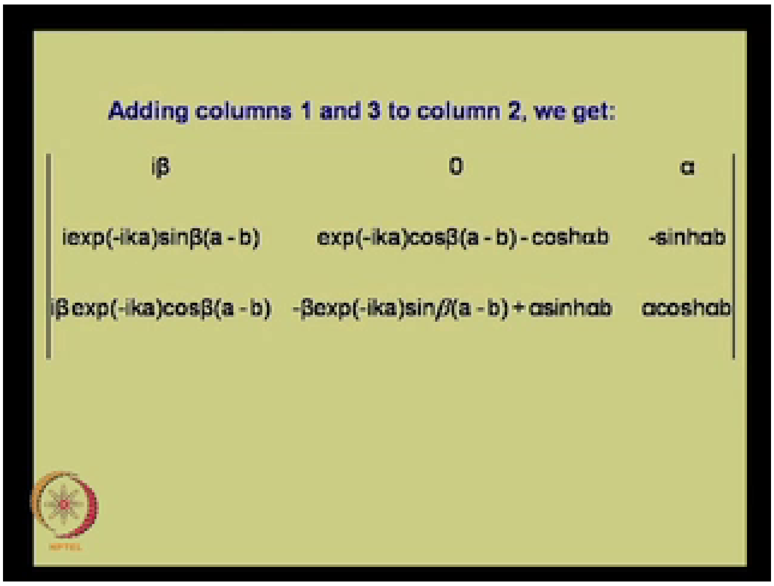
So, I just put those terms down here, so it is now 3 by 3 determinant and the factor in term and the front is minus 1 power 1 plus 2, because we have the subscript 1 1 and 2. So, we will affectively get a minus 1 here, but please remember again, this determinant is still evaluating to 0, we are still evaluating the same determinant, our originally determinant was said to evaluate to 0 and we are simply proceeding along those same same lines.

(Refer Slide Time: 33:16)



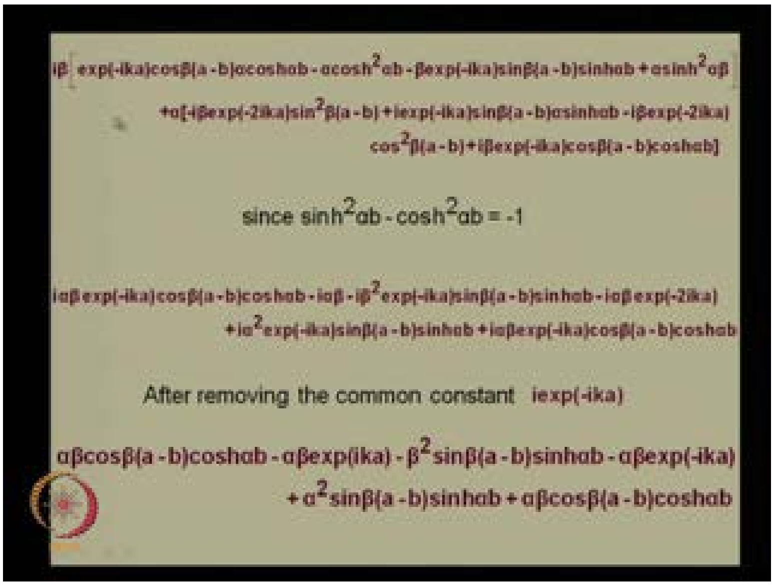
So, since that determinant must evaluate to 0, we can ignore the constant minus 1 power 3, as well as the multiplicative factor 2 in column 1 as well as in column 3 right. So, there is the multiplicative factor here, and the multiplicative factor here, we can ignore this, we can remove this 2, and we get the remove this 2, all the 2's here and so we the determinant now becomes something that we, that is of the form that is shown here. So, it is a 3 by 3 determinant, so it is much easier to evaluate. So, again we play a little bit, because they can see here and i beta here and alpha and the minus alpha and alpha minus i theta here, so it gives us root 2.

(Refer Slide Time: 33:51)



Further simplify, so we simply add column 1 and column 3 to column 2. So, if you do that, the top term become 0 and the terms here become the, what you see here and you can see, I have got the hyperbolic function here. So, that incorporates and at different locations, you see the hyperbolic function, and that incorporates there is the fact that we had those terms that, we had that e power x plus or minus e power minus x. So, that is how we got this.

(Refer Slide Time: 34:17)

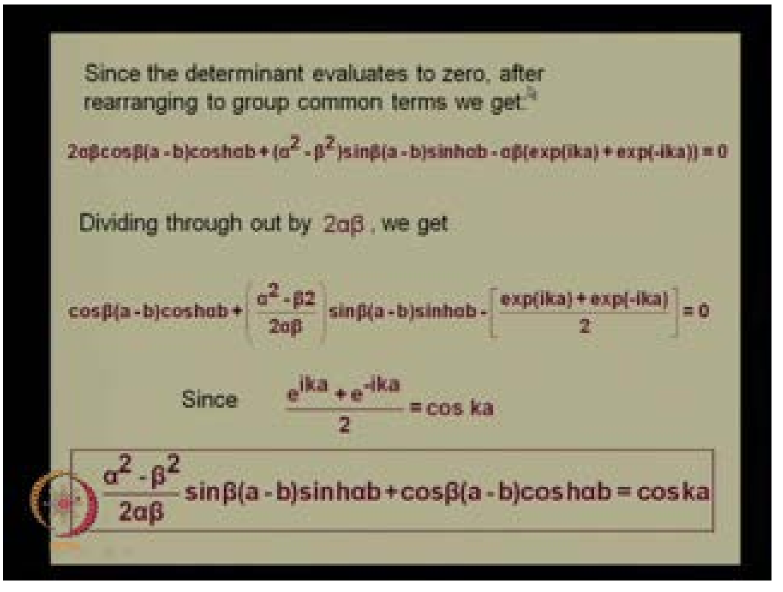


So, now we can expand this determinant. So, expanding it we get i beta times this big term here plus alpha times this big term here. So, I as I mentioned I suggest that you go ahead and try this out, because it values straight forward if you go through it once, you will feel very comfortable that you understand how this energy gaps comes. So, it is simply i beta, this time this, minus this time this, that is the first term and then alpha and we will have this time this minus this time this. So, that is all we are going to do and so, that is what you see here, this being expression here.

In this expression, we can take advantage of this mathematical identity, just like you have sin square theta plus cos square theta equals 1. If you take the hyperbolic functions, sin hyperbolic square of some theta minus cos hyperbolic square of the same theta is minus 1. So, if you put minus 1 correspondingly here, so you have a, you have similar terms here, you see here cos square alpha beta and sin square alpha beta, so you are in sin hyperbolic and cos hyperbolic. So, you can simplify it, you get this expression that is out here, much simplified expression begins to appear here, again we can remove the constant common constant i exponent minus i k a, you will find that showing up in all the terms. So, you can remove this constant and since it evaluates to 0, you can do that.

So, please note all a along we are now now expanded this determinant and it is equal to 0. So, you can remove multiplicative constant, so we can remove this. Therefore, the expression we end up getting is what you see here. So, this is the expression that you rand up getting, after you do these two simplifications, we have expanded that you determinant, incorporative this simplification and incorporated this simplification, you got this equation that you see here.

(Refer Slide Time: 36:03)



Now, since the determinant evaluates to 0, we can regroup the term, common terms we get and so, we have and we we can rewrite it in in this form. So, this is what we have done and we can divide throughout by 2 alpha beta, we see at two alpha beta here. So, we can this device throughout by 2 alpha beta. If you do that, we get this expression cos beta a minus b cos hyperbolic alpha beta alpha b alpha square minus actually this is beta square here by 2 alpha beta and you have this terms here equal to 0. So, this is the equation that we get, and since e power i k a plus e power minus i k a by 2 is cos k a, we can correspondingly convert this to cos k a. So, that is that is how we get the cos (( )) system. So, the equation is now this, what you see here. So, this whole thing was equal to

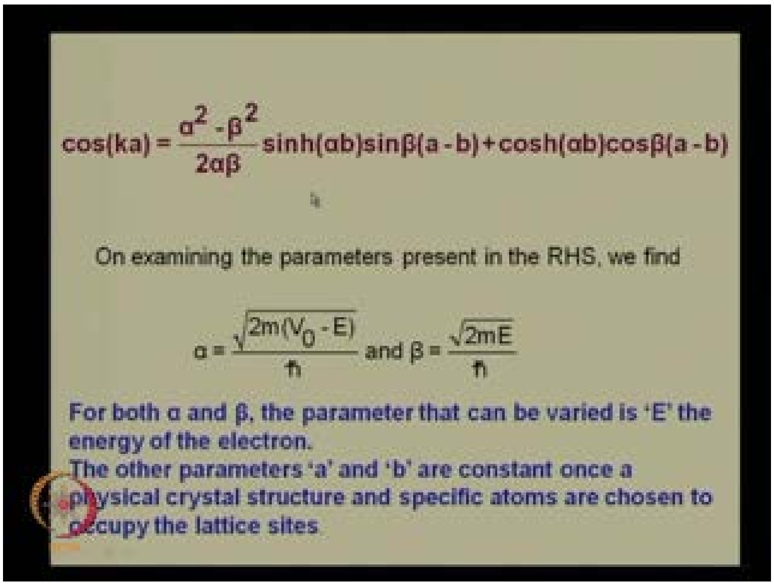
0, you will just this is equal to cos k a. So, the cos k a can come to this side and therefore, we get this equation, so this is the equation that we get.

So, now let us re assess what we have done, we have got a equation where we have alpha, we have beta and these are system constants. So, where we basically have a some, but it has energy, both of them have energy incorporated in them, this as energy incorporated in it, this has energy incorporated in it.

So, one has a V naught minus e terms, the other has the e terms, so both of them have energy incorporated in them, this a and b are system constant, in the sense a is the periodicity of the system, b is the distance between those potential wells. So, that is incorporated here, so that is something that is fixed for the system. So, we do not have any variation in there and so, affectively in this entire equation, what we have that can vary is the wave vector and the energy values that you have available in this system.

So, that is what we can change, we can look at various energy values and so on. So, we have an expression on the left hand side of this equation, and we have a expression on the right hand side of the equation.

(Refer Slide Time: 38:06)



So, I just rewritten this equation, I just (()) it around. So, this is cos k a here and the entire expression that we just came up with this now written on the side. So, as I mentioned, on examining the para parameter present on the right hand side to the equation, alpha as this parameter here, h bar is the constant, m is the constant and V naught is the constant, energy is something that we can explore, we can try out the various energy values and therefore, various alpha values we can get. Similarly, in beta m is the constant, h bar is the constant, and various values of energy we can try out, these two came from out original solution of the Schrodinger wave equation.

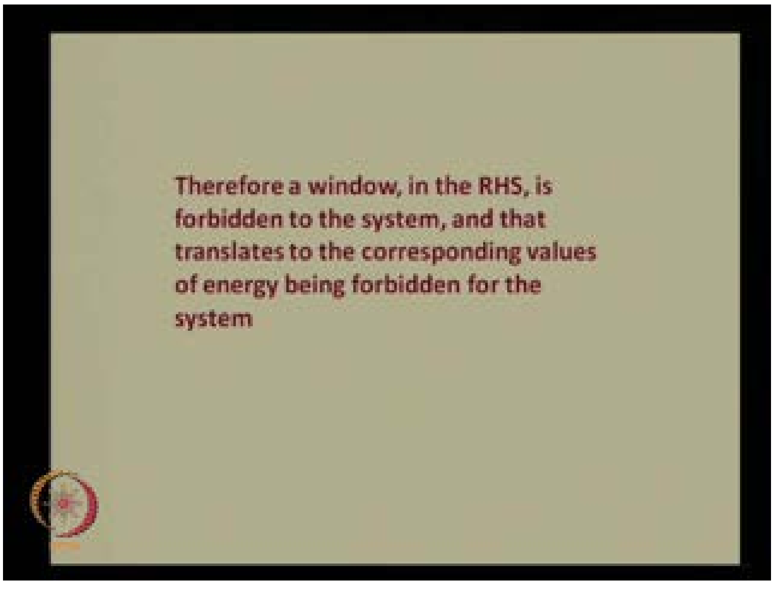
So, for both the parameters alpha and beta, the parameter that can be varied is e, the energy of the electron that we are examine, other parameters a and b are constant once of physical crystal structure and specific atoms are chosen to occupy those lattices.

So, that is all fixed, so what you will find is, if you actually evaluated this equation for a variety of a possibilities of of energy values on the right hand side, this expression on the right hand side can will give you series of values, corresponding to this at expression; on the left hand side we have cos k a. By virtue of its the fact that it trigonometric function cos k a, we know that this cos value can only be between plus or minus 1. So, we cannot be outside this window, it has to stay with in plus or minus 1 window.

What we will find is, the based on the energy values you choose, this entire expression here will on several occassions fall within the plus or minus 1 window, and on some occassions it will this expression on their right hand will evaluate to values which are greater than this plus or minus 1 window. So, you will have, you may have a safe for the example of 1.5, this expression will evaluate to say value of 1.2, 1.5 or some such thing first specific values of energy.

So, that therefore, it gives us the situation where this is becomes an (()) relationship are in inconsistent relationship. So, this is interpreted to indicate that values of energy where the expression of the right hand side stays within the plus or minus 1 window which is required based on the the expression on the left hand side, those are values of energy that are now allowed for the system, though those values of energy therefore on the band gap sorry they form the allowed energy band of the system. The other values of energy where this expression here evaluates to to numbers which are outside this plus or minus 1 window and therefore, to to values that are (()) or inconsistent with the left hand side, those values of energy now represent forbidden energy values or band gaps.

(Refer Slide Time: 40:43)



So, that is how we evaluate this equation, therefore so, in other words we say here therefore, a window in the RHS is forbidden to the system and that translates to corresponding values of energy being forbidden for the system. So, there is specific values of energy corresponding to this right hand side, specific values of energy that we can try on this right hand side, because those that is the only real variable that we have the right hand side, we can try values of energy which will give us values that are in consistent to the left hand side with the requirement of the left hand side that will be between plus or minus 1.

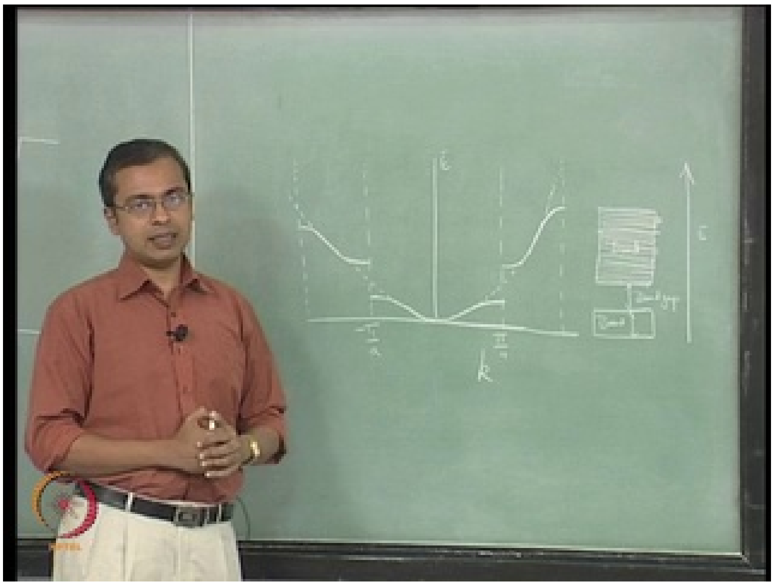
So, we are able to see that, so this is the conclusion that we we were interested in, this is the information that we were interested in. So, all those solving the determinant we could have continued on the process and try to get ourselves (( )) values for the capital A, capital B, capital C and capital D, we have not actually done that, we have used that the framework, we have used that determinant that comes out of that process to give ourselves this equation that you see on the screen so that the equation now tells us what are allowed values of energy, and what are not allowed values of a energy in this system.

So, starting with the system where we had a periodic stricture, we are able to actually look at the constraints placed on the system and incorporate the constraints in the Schrodinger wave equation, and in that process we have actually gone ahead and looked at the value of that Schrodinger, this solutions to those Schrodinger wave equation under conditions where the potential is 0 and the potential is v 0.

Taking this conditions together we have compare the value of the wave function at are at the origin as well as at at a periodic boundary, and based on the periodic boundary requirement at two other locations. And then we have compared both, we have set that know the solution have to reasonable, therefore the value of the function on either side of those locations has to be the same, and the value of the the derivative on either side of to those locations has to be the same, this give us four equation we attempted to solve those four equations and we found that we had a very nice interesting solution coming as the result of that process.

So, what we have seen in the this class to summarize is that, we have actually looked at, how we can evaluate based on the constraints placed on the system, how we can evaluate and see what are values of energy that are allowed in the system, and what are values of energy that are forbidden in the system. And therefore, something that we drew pictorially in are previous class, where we previously prove something pictorially is something that we are now able to come up with us in terms of numbers. So, we will briefly see this on the board as we wind up this class.

(Refer Slide Time: 43:32)



So, we saw in in our last class that we we basically could draw energy verses k and then at the Brillouin zone boundaries. So, this is minus pi by a and plus pi by a, we found that the electron parabola was getting distorted.

So, we found that it actually showed a behavior that look like this. So, if you draw the next Brillouin zone, we just to 1, 2 Brillouin zone and we could be done. So, if you look at this, this is how it would be (No audio from 44:17 to 44:32). And in this context we designated this to be a band, allowed energy band, this was a forbidden band gap and this was other allowed energy band. So, now, so this is how we were able to see this pictorially, we have now been able to do calculation which at which tell us in this energy scale, what is this set of values of energy that are allowed, so therefore, what is the allowed band and what is this set of energy values that are forbidden and therefore, the band gap and then we can the next band.

So, that is the calculation that we have done. So, we have we able to actually understand this system in a very in a pictorial sense, you also able to understand the sense system in a detailed calculation based sense, using all the (()) mechanical details that we would have to impose on this system. So, we have a got lot of information about this system, we now understand how bands are originate with the system, we in in a high school we are simply told accept that there are bands, and for the most, part many of the things that we have material usage that we do that is the information that we require, we simply need to know what the band gap is and many material properties we can say on that basis, or now we are able to see what is the basis what is the fundamental reason, why a band exist in a material.

This as something that we have not look at, before we were not aware of before. I will also high light one more thing. I mentioned that I mention this several times that you know this looks like a continuous curve, but it several discrete points. And so, this is simply means that this band is the series of discrete energy levels that are allowed, a very very very closely space, relative to the band gap values or even the band extend of the band. So, please always keep that in mind, this is series of discrete energy level which are extremely closed space and that you have the band gap.

So, we have now understood the origin of bands in a material and this picture also a a we will see later helps of, will also help us the understand the un isotropy in materials. So, we have taken lot of information, brought it all together here. In our next class, we will look at utility of this information and more insides that we can gain in to the materials based on all those we have understood so far. So, with that we will halt for today, we will take it in the next class, thank you.