Introduction to Quantum Mechanics
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Lecture - 03
Numerical solution of a one dimensional Schroedinger equation for bound states- I

In the previous 2 lectures, we have considered 2 cases; one of a particle moving in a delta function potential and particle moving in a finite size box for which the Schrodinger equation could be solved analytically; however, all potentials are not; I mean able to see this kind of treatment.

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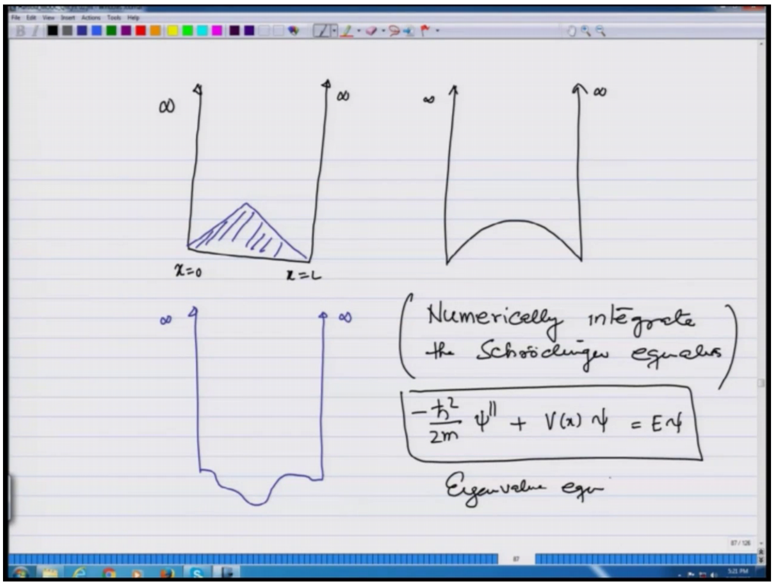

For example, even if I take a potential where the potential becomes infinity at the boundaries let us say x equal 0 and x equals l, but change the potential in between suppose this like this or in the potential which is like this or in general a potential which is some arbitrary shape in between how do I solve the Schrodinger equation and for that we have to numerically integrate the Schrodinger equation, how do I numerically integrate at differential equation, I will write now focus principally on solving the Schrodinger equation which is a second order differential equation psi double prime plus V x psi equals e psi and this is an Eigen value equation; that means, I have to satisfy certain boundary conditions then only the solution is acceptable.

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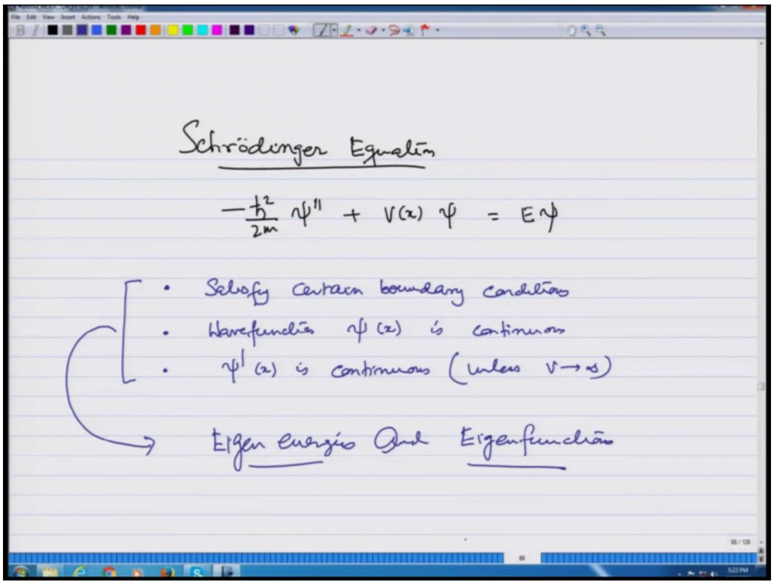

So, let me just give you that for the Schrodinger equation minus h cross square over 2 m psi double prime plus V x psi equals E psi I am supposed to number 1 satisfy certain boundary conditions the wave function psi x is continuous and third psi prime x is continuous unless we goes to infinity, I have to satisfy all these 3 conditions and then this together gives me the Eigen energies and eigenfunctions.

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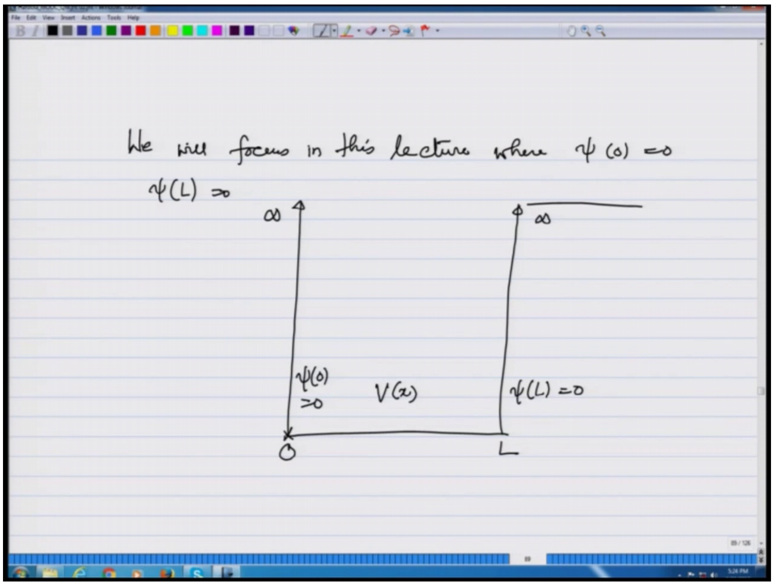

So, what we need to do is solve this equation satisfying the boundary conditions and making sure that psi n psi prime both are continuous to start learning about numerical techniques we will focus in this lecture on a simpler problem where psi 0 is 0 and psi L is 0 that will also make us understand the problem better.

So, this is the problem with infinite (Refer Time: 04:24) high was V goes to infinity at 2 points and remains infinity outside between 0 and L, V is some shape V x. So, psi is 0 at this edge and psi as 0 at the other edge and we have to build the solution in between. So, in numerical solution of differential equations we actually construct the solution how do we do that? We start integrating the psi prime and psi double prime to update our size and all that.

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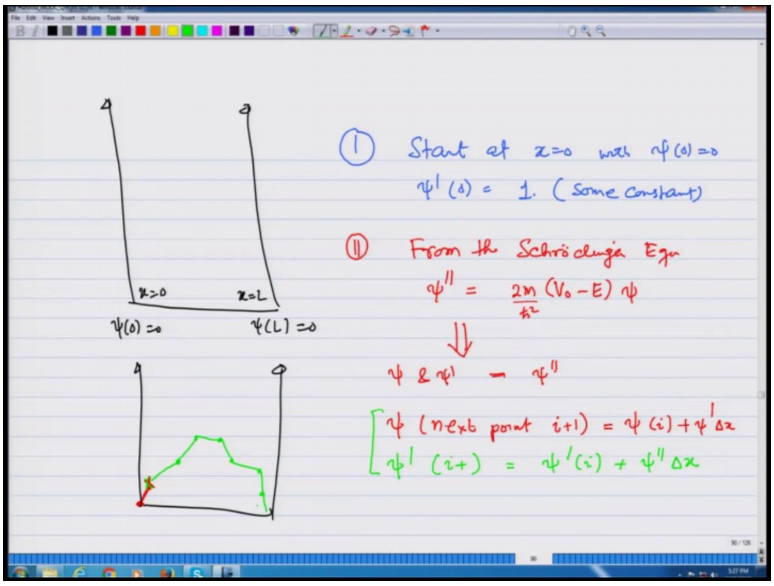

So, one technique could be in this case in which case the psi 0 on 2 sides psi 0 and psi L both are 0 this is x equals 0 x equals L. So, one way of constructing could be start at x equal to 0 with psi 0 equals 0 and psi prime 0 equals some finite number let us say 1 or some constant.

I will keep showing what I am doing here. So, in this box, I have let me show psi by red psi equals 0 and some slope what we can do with this is find the value at the next point. So, number 2 from the Schrodinger equation psi double prime is equal to V 0 minus E 2 m over h cross square times psi. So, I know this implies that at any point I know psi and psi prime, it gives me psi double prime also. So, from this point, on the left hand side started x equal to 0, I have update it and so I can write psi at the next point, let me call it i plus 1 th point is equal to psi at point i plus psi prime delta x and I can also update psi prime at i plus 1 th point as psi prime at i th point plus psi double prime delta x and how do I know psi double point of I know psi x some point I know psi double prime also.

Once I do that. So, I found everything on this cross from here I again build my solution to the next point and from that to the next point, from that to the next point, from that to the next point and so on, I can keep building the solution because I am keeping terms only up to the first order, I have to make sure that this delta x is really small in the second order can be neglected now once we start with this process.

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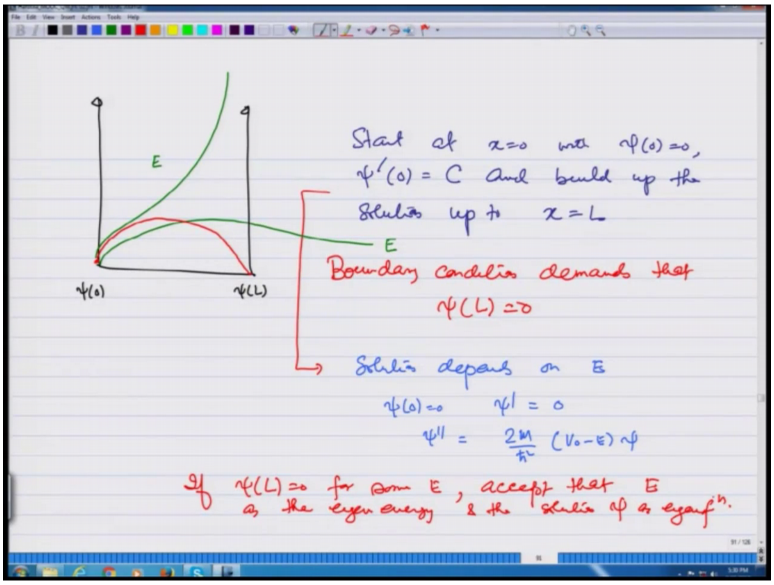

So, in this case, I am taking the case where the psi vanishes on both sides psi equals 0 psi equals L. So, start at x equal to 0 with psi 0 equals 0 psi prime 0 equals some constant. So, let us write it C, I wrote one earlier and build up the solution up to x equals L. Now boundary condition demands that psi L be equal to 0, remember now when I am starting from psi equal to psi at x equals 0, I am building up a solution and the solution depends on E; what is that happened because I had a psi 0 equal to 0 psi prime equal to 0, but I have psi double prime at any point which is given as 2 m over h cross square V 0 minus E psi.

So, depending on what; E is psi prime is given and I use all these 3 to build up my solution. So, psi L is not going to be 0 until I really have that Eigen value. So, what could happen? For example, if I build up the solution one solution could be like this, I am showing in green this is not acceptable. So, this is some e second solution go to do like this some other e unless I have exactly write E that at least goes to 0 on the other side and that is acceptable. So, if psi L is equal to 0 for some E accept that E as the Eigen energy and the solution psi as Eigen function and then you can keep increasing E and find more and more and more states. Since the particle is bound in this case between 0 and l; that means, V goes to infinity outside this boundary there going to be infinite number of states in this case and so you can keep scanning over E and find more and more states.

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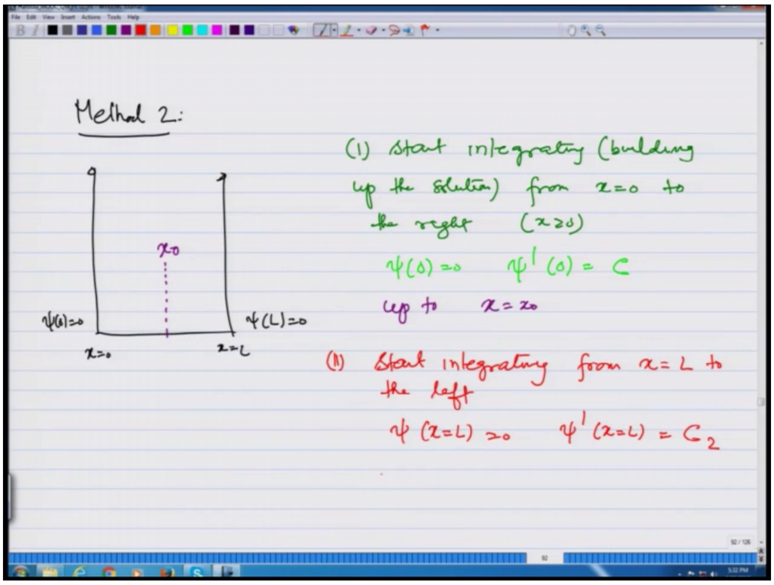

The other method could be again using the property is the solution is the Schrodinger equation and this case again I have psi 0 equals 0 psi L equals 0 x equals 0 x equals L number 1 start integrating or what I say building up the solution from x equals 0 to the right, where write means x greater than 0. So, you start with psi 0 equal 0 psi prime 0 equals sum number and then you know psi double prime from psi and you start integrating out up to certain point x, let us call it x 0 up to x equals x 0 second start integrating again building up solution from x equals L to the left. So, what you will do is psi at x equals L is 0 take psi prime at x equals L to be some other constant C to psi double prime I know.

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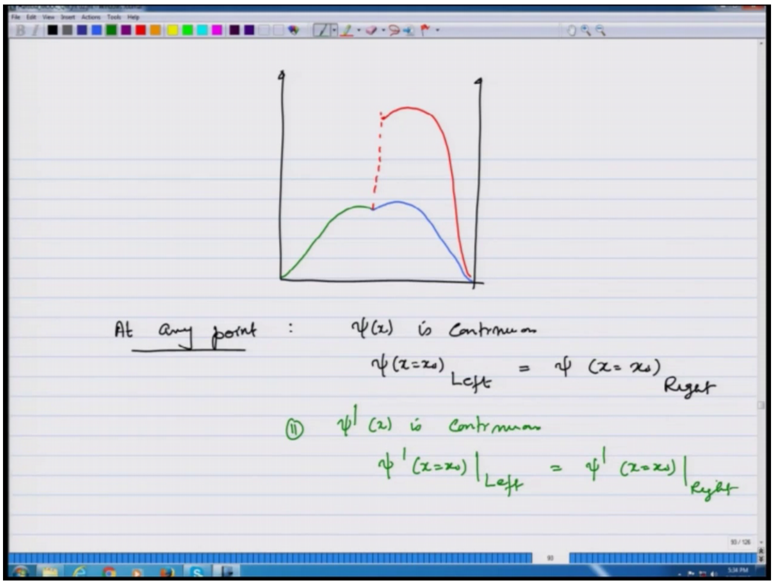

So, you start again integrating to the left and up to x equals x 0. So, what I have we done what we have done is in this potential, we will started a building up a solution from here, let us say this is what comes out from this side and we started building up the solution from the right side and let us say this comes out like this it need not match the other situation could be that let me show it in red this fellow could be like this what we should do is at x equals x naught the solution should match what does that mean at any point what do we have for the acceptable solution psi x is continuous; that means, psi x equals x 0 from left should be equal to psi x equals x 0 from right and number 2 psi prime x is continuous. So, you should have psi prime x equals x 0 from the left is equal to psi prime x equals x 0 coming from the right.

So, what you could do is match the 2 solutions was by multiplying by a factor and then compare the psi prime values.

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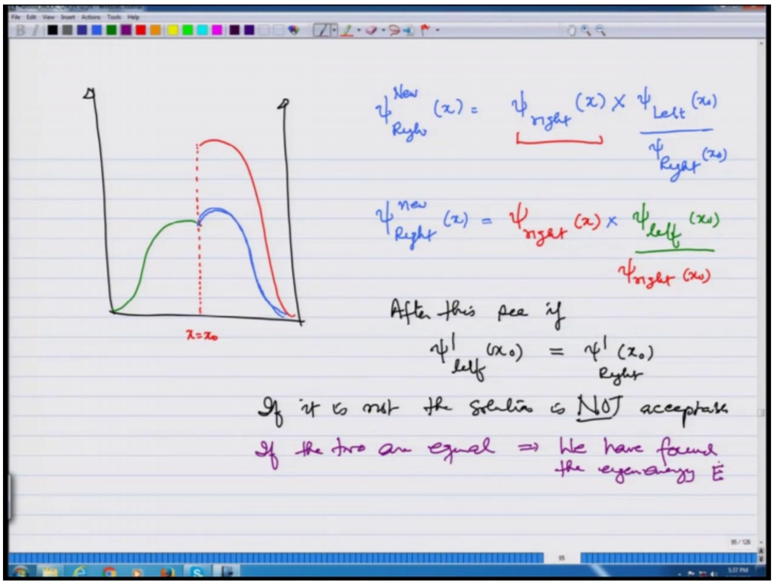

So, again let me make this picture and you have a solution coming from the left it could be like this solution coming from the right which could be like this. Now let us see if it at this point where we are matching which is x equals x 0. Since we started with different slopes first the wave function did not match. So, what we need to do is multiply the right hand side to the factor that brings it down makes the wave function match at this point. So, I can write psi right at x, I could write as psi right at x times psi left at x 0 divided by psi right at x 0, this will make the match. So, this will make it make the curve to be this blue one right. So, let me write this new.

So, from red we have done this one let me write this one as red. So, I have made psi right new x equals psi right x times psi left x 0 divided by psi right x 0 and then after that this is step one and after this, this C if psi prime left x 0 is same as psi prime x 0 coming from right if it is not the solution is not acceptable on the other hand if the 2 are equal then we have found the Eigen energy E. So, for some energy they are equal and that is Eigen energy they will not be equal for all energies after all this rescaling has been done.

So, this the way to find Eigen value and the eigenfunction in 2 different ways one by making sure that the wave function is smooth all over; that means, psi and psi prime are the same no matter which side I integrate the wave function form and the other I build us smooth wave function starting from one boundary and make sure that the other boundary condition is also satisfied both are acceptable ways.

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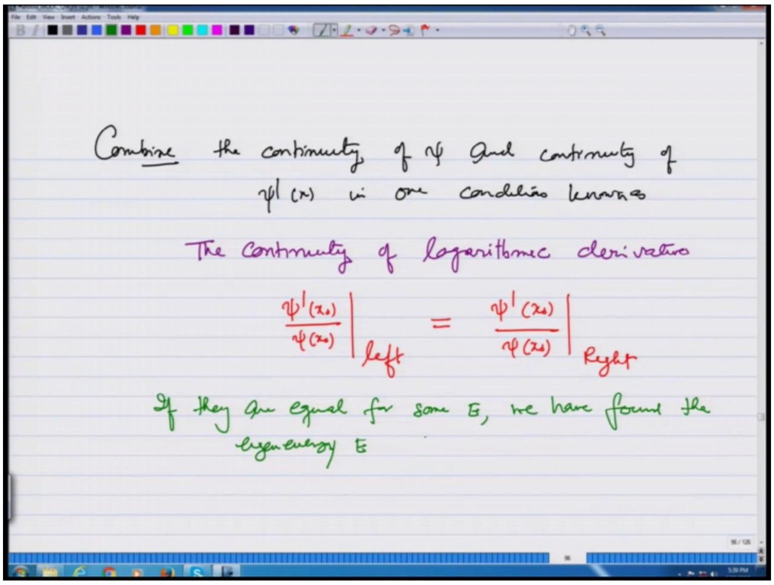

Now, we sometimes combine in fact not some time all the time combine the continuity of psi and continuity of psi prime x in one condition known as a continuity of logarithmic derivative. So, in this case what I do is I take psi prime x 0 over psi x 0 left and compare this with psi prime x 0 over psi x 0 coming from right and check if they are equal if they are equal for some e we have found the Eigen energy E, if not we again go to some other energy and check.

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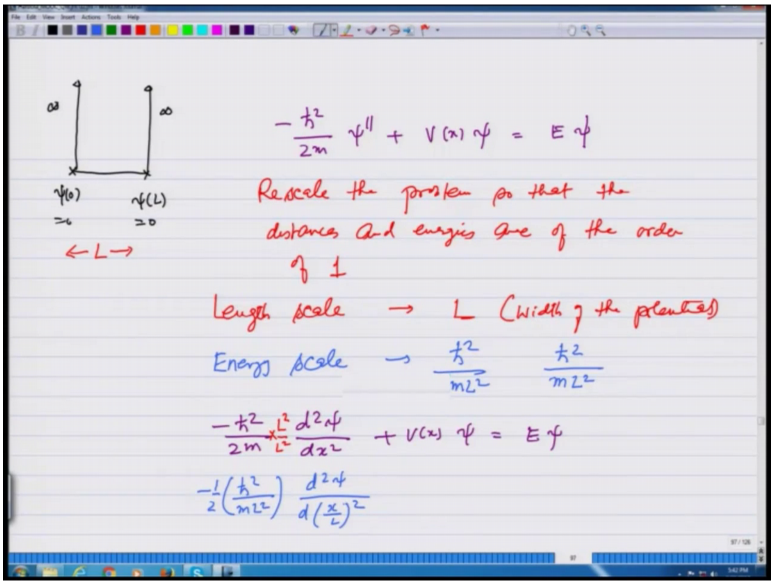

So, we can scan over the energy and see what happens. So, these are going to be the 2 methods which we use in calculating the eigenfunctions and Eigen energies of a given problem a right now as I said earlier we have occurring on problems where the potential could be anything between x equals 0 and x equals l, but it is going to be infinity outside that region. So, that wave function is always going to be 0 at the 2 boundaries now the Schrodinger equation is minus x cross square over 2 n psi double prime plus V x psi equals E psi. Now these numbers h cross and m are very small we are dealing with microscopic world. So, is good idea to rescale the problem? So, that the distances and energies are of the order of one; that means, we changing units rather than of the order of being 10 days to minus 36; 10 days to minus 19 and so on that will be very difficult to program in a computer.

So, what we do for example, in this case in the case of the problems that we are dealing with right now is that length scale we will take to be L that is the width of the potential and the energy scale naturally becomes h cross square over ml square. So, with keep the lens scale to be h cross square over ml square which is dimensionally correct. So, let us rewrite the Schrodinger equation for this. So, when we do that we have minus h cross square over 2 m d 2 psi over d x square plus V x psi equals e psi let me multiply here by L here and divide by L square. So, that I have the equation as minus h cross square over m L square one half in front d 2 psi over d of x over L square plus V x psi x equals e psi divide.

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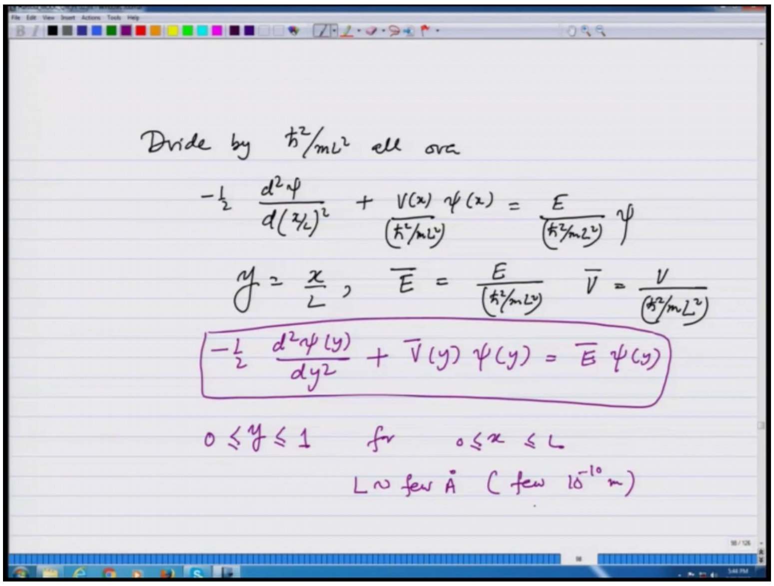

By h cross square over ml square all over to get minus half d 2 psi over d x over L square plus V x psi x is divide by h cross square over ml square is equal to E over h cross square over m L square psi call y equals x over L and E bar equals E over h cross over m L square and V bar equals V over h cross square over m L square to rewrite the equation as minus half d 2 psi as a function of y over d y square plus V bar y psi y equals E bar psi y and that is my equation in this dimension less quantities y E bar and V bar. And now I can take y between 0 and 1 for x varying between 0 and L.

Remember in quantum mechanics or in atomic quantities L is of the order of may be a few young storms which is few 10 raise to minus 10 meters. Now I can vary y between 0 and 1. So, I can take the increment in y to be of the order of point 1 and so on where as if I want to do the same thing in terms of x it would be much more difficult and numerically unstable.

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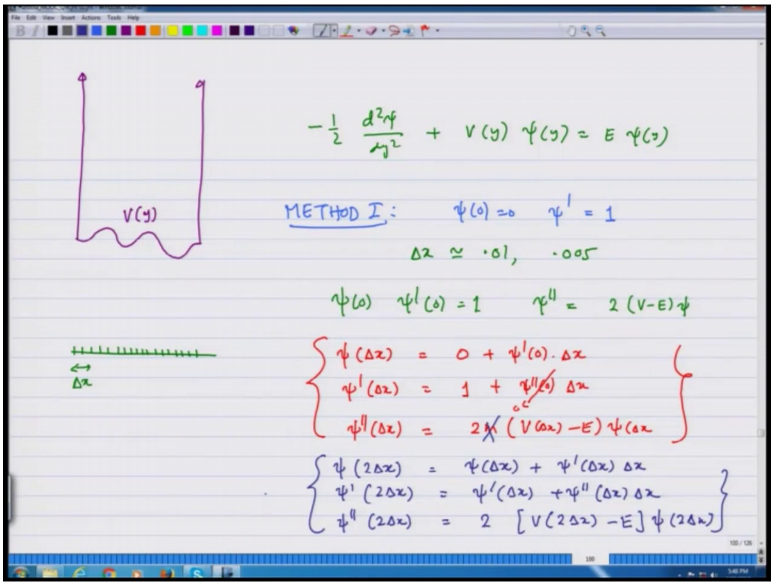

So, now we are able to integrate the equation. So, I have again I will take this box where in between there some potential let us call it we now y this is given in units of h cross square over m L square. So, I am going to drop that bar in this write this as minus 1 half d 2 psi over d y squared plus V y psi y equals e psi y method one is going to be number what we did we start with psi as 0 equals 0 take psi prime equals some number let us take it to be one and then integrate. So, what we will do is we will divide this whole thing into small e of interval delta x. So, delta x could be of the order of point o 1.005 over so on, right some delta x very small number.

So, I will start from psi equal to 0 and psi prime at 0 equals 1 psi double prime by the Schrodinger equation which is 2 V minus E psi, then I have psi at delta x would be 0 plus psi prime at 0 times delta x psi prime at delta x is 1 plus psi double prime at 0 which is 0, right. Now delta x and now I can write psi double prime at delta x to be equal to 2 m V at delta x minus e times psi at delta x. This is one cycle completed from here I can go to the next step and write psi 2 delta x would be equal to psi delta x plus psi prime delta x delta x psi prime 2 delta x is equal to psi prime at delta x plus psi double prime which we have already calculated at delta x delta x and psi prime 2 delta x is now updated to be equal to 2 V at 2 delta x minus E psi at 2 delta x.

This is another cycle we have completed this m should be way away and now I can build up the solution and so on.

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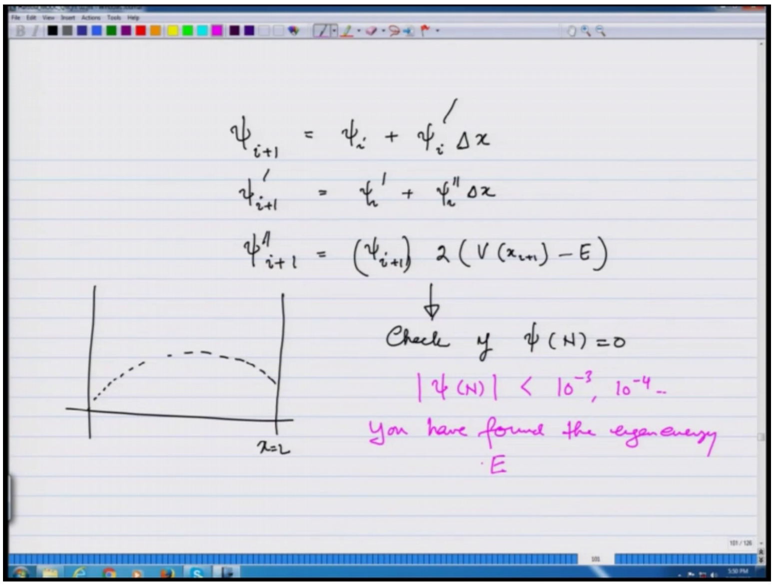

So, in general what I am doing is I am writing psi at i plus 1 th point to be equal to psi at i plus psi at i prime times delta x, I am updating psi prime at i plus 1 as psi i prime plus psi i double prime delta x and once I found psi at i plus I can update i psi double prime here plus 1 is equal to psi at i plus 1 times 2 V at x i plus 1 minus E notice that we will depend on E and this way I can go all the way building up the solution at different points all the way to the other side x equals L and then check if psi let us say the last point is n is equal to 0 and numerically it is very difficult to make sure is 0.

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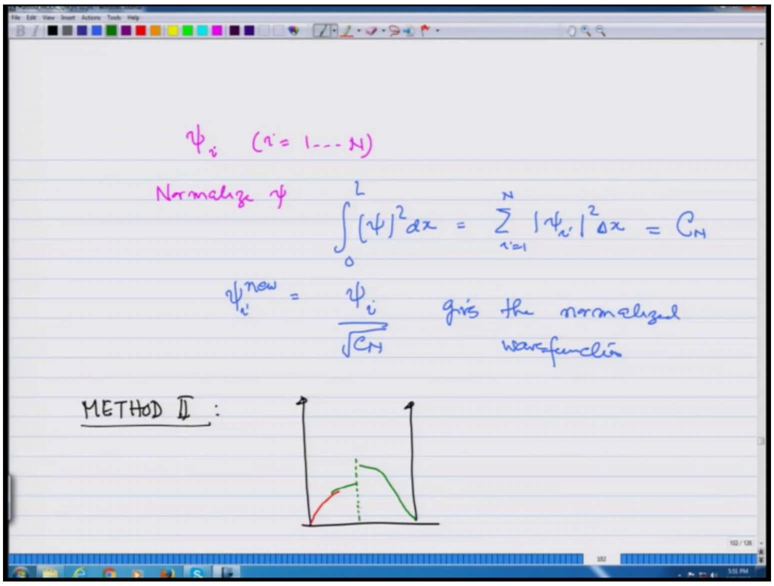

So, what you do is you say psi n modulus is less than some very small number let us say 10 raise to minus 3 or 10 raise to minus 4 or so on if that is the case you accept it. So, the moment that happens you have fund the Eigen energy E whichever E that happens for your found that energy and once you have found that energy you have also found psi i at different is i equals 1 through n gives you the value of psi at each point. So, now, you normalize psi what you do you calculate integral psi mod square d x 0 to L which will be nothing, but summation i mod psi square delta x i equals 1 through n and this gives you sum number let us say C n then psi i new is equal to whatever psi you calculated earlier divided by square root of C n give the normalized wave function that is one way of finding the wave function in this case.

Method 2 which in this case is not will required, but I am giving it because it will require for cases that will discuss in the coming lectures. In method 2, you actually start building up the solution from one side you start building up the solution from the other side and you match a logarithmic derivative at some point x 0 once that matches that gives you the Eigen value.

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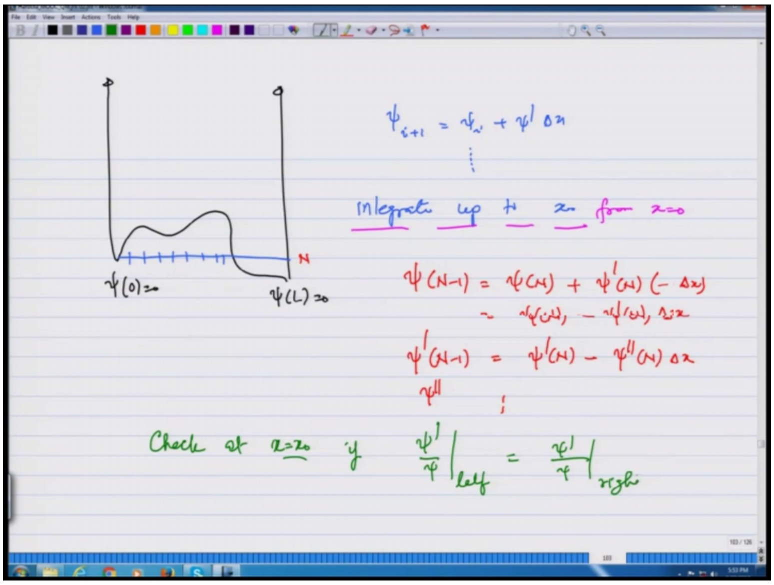

So, what you do is some potential in between we have psi L equal to 0 psi 0 equals 0. So, you start you again divide this whole thing into small-small-small intervals. So, you write psi i plus 1 equal psi i plus psi prime delta x and all those steps that we did earlier and integrate up to x 0 from x equal to 0 this done that is the last point is n, then you go psi n minus 1 equals psi n which is 0 plus psi prime n times minus delta x because you going left.

So, this is going to be psi n minus psi prime n whatever value you assume times delta x you go psi prime n minus one equals psi prime at n minus psi double prime n delta x and then to update psi double prime and so on. So, you build up the solution the other way and then check at x equals x 0 if psi prime over psi left same as psi prime over psi right how do we check that we can say that psi prime over psi left minus psi prime over psi, right, modulus is some less than 10 raise to minus 3 or 10 raise to minus 4 that you have to play around and see where you get the answer once that happens if it happens for certain E that is the Eigen value.

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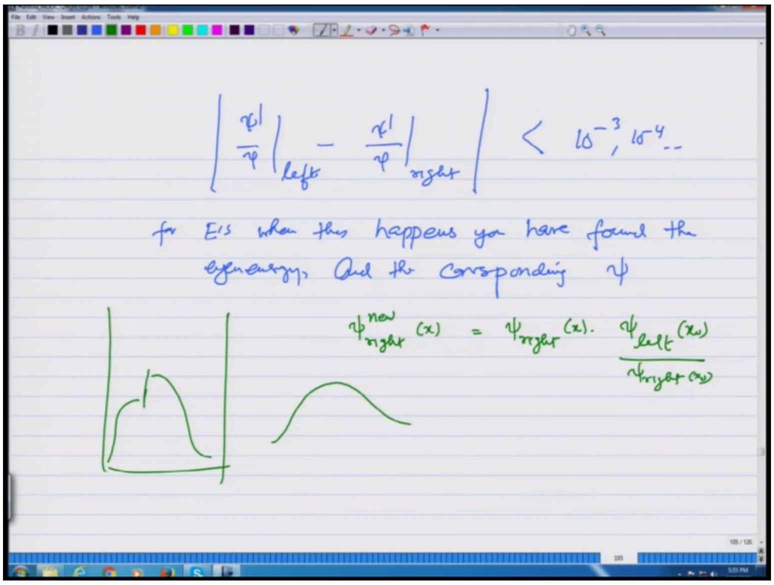

So, for E s when this happens you have found the Eigen energy and the corresponding psi not to make the psi proper what you do is you come from left you come from right. So, what you do is psi right at some x new has to be equal to psi right at x times psi left at x 0 to at website right at x 0 this will make sure that now the way function match at x equals x 0 and then you found the continuous wave function and in the normalized. So, what I have given you is in this very specific kind of problem where the wave function vanishes at the 2 boundaries how to find the wave function and the Eigen energies.

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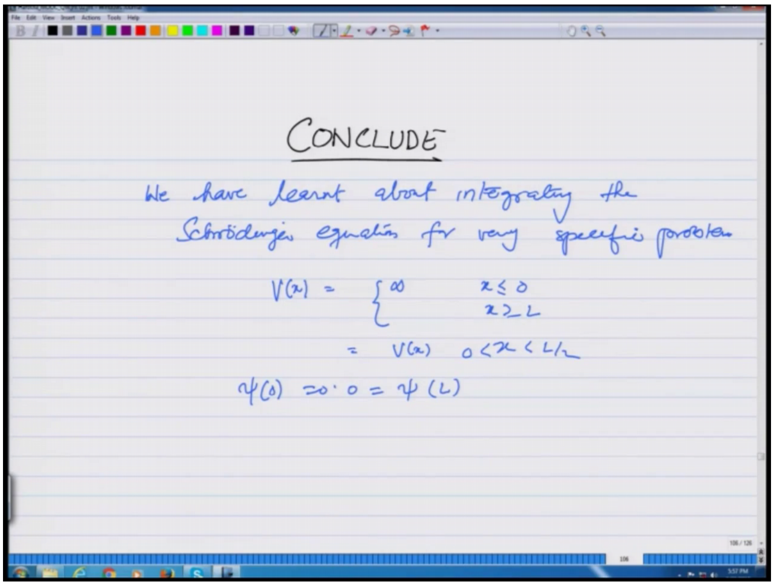

So, to conclude we have learnt about integrating the Schrodinger equation for very specific problem where V x is equal to infinity for x less than equal to 0 and x greater than equal to L and is equal to V x for x in between.

So, psi 0 is 0 and so is psi L and we found a way of finding the solution, we will now in the next lecture consider cases where psi it is not vanishes at these boundaries, but goes all the way to infinity out find solutions for those situation.