Introduction to Quantum Mechanics
Prof. Manoj Kumar Harbola
Department of Physics
Indian Institute of Technology, Kanpur

Lecture - 04
Numerical solution of a one dimensional Schroendinger equation for bound states- II

So, in the previous lecture you had learnt about Numerical Solution of one-dimensional Schrodinger equation.

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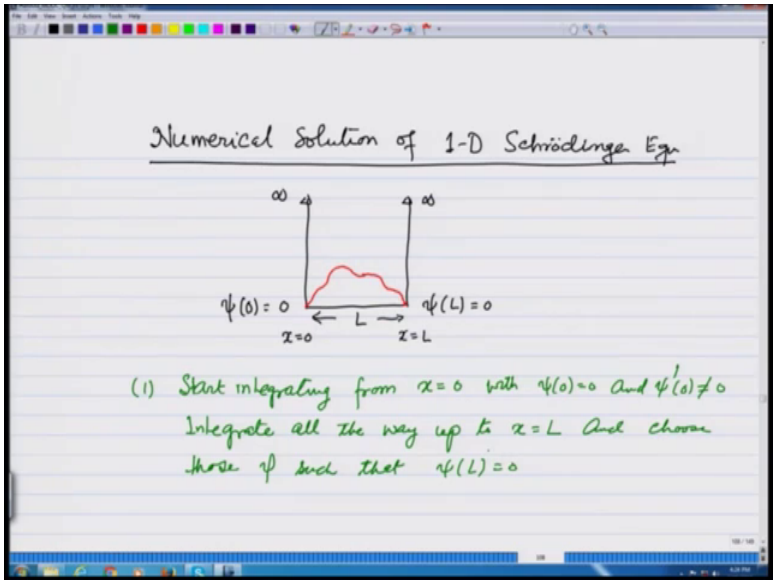

And this was a very specific kind of Schrodinger equation where we had said that the potential goes to infinity at some reasonable small distance L so that the wave function psi at the two edges which I denote as x equals 0 and x equals L they are both 0. So, this is x equals 0 and x equals L. In between the potential varies the wave function could be anything in between, but it goes to 0 at the 2 ends. We had learnt two methods one was start integrating form x equals 0 with psi 0 equals 0 and psi prime 0 some nonzero value integrate all the way up to x equals L and choose those psi's such that psi L equals 0 and that is an eigen function.

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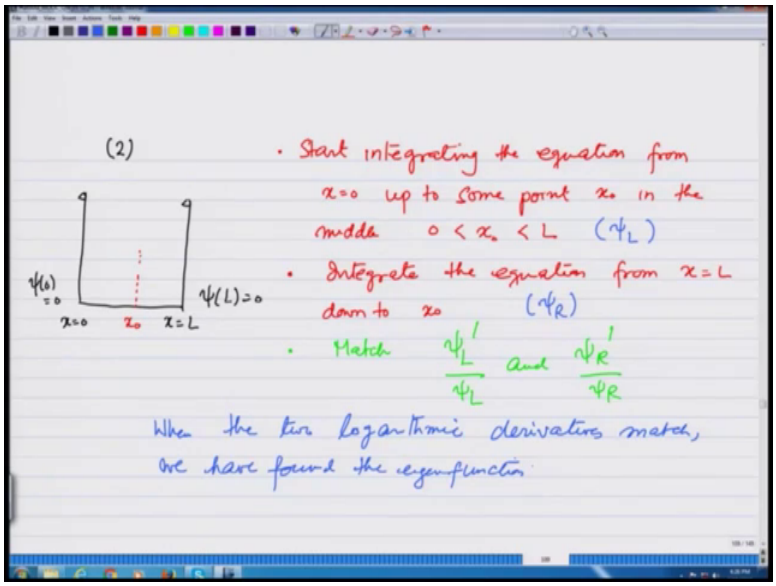

The other method that we had talked about was, let me make this picture again x equals 0 x equals L psi L is 0 psi 0 is 0. The other method was start integrating the equation and when I say integrating I mean I am doing numerical integration from x equals 0 up to some point x 0 in the middle. So, somewhere I choose a point x 0 well. So, x 0 is greater than 0 less than L number 1.

Number 2 integrate the equation from x equals L down to down to I mean you are going to the left x 0 and third step was match psi left prime over psi L and psi right prime over psi right. While left or right I mean this solution gave me psi left this gave me psi right and then I match this when the 2 logarithmic derivatives match we have found the eigen function.

So, this is what we did in the previous lecture. What you want to do in this lecture is go to a general case where the potential does not go to infinity at x equals 0 and x equals L. So, the case we are considering now, is a general potential and if you make it just to give you an idea this is x and I am plotting v x for example, it could be some potential like this more regular potentials could be for example, a potential increasing linearly on 2 sides this is v x this is x.

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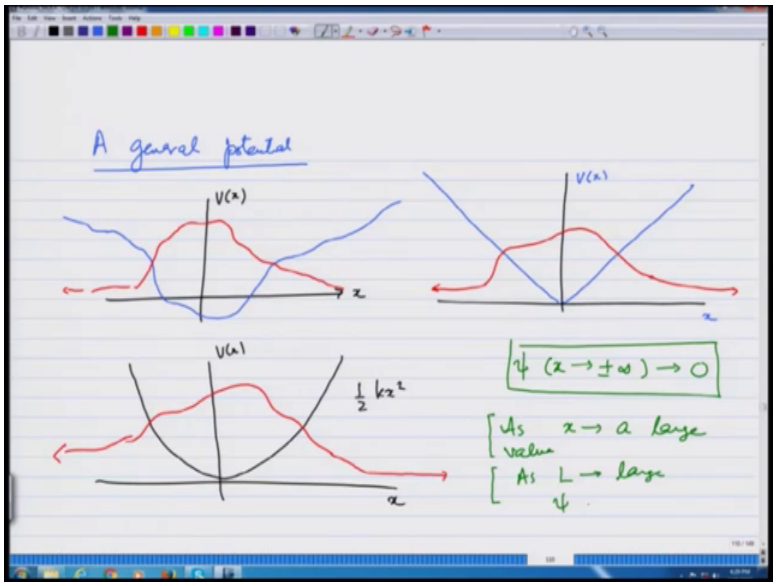

Another example that you have already seen and we have solved it analytically and it proved to be a good case study to check our numerical techniques is the harmonic oscillator potential one half k x square. In all these case what is going to happen is that the wave function is going to be concentrated near the origin of where the potential is deepest and go to 0 as you reach distance very far along the x axis. So, in these cases what is happening is psi x going to plus or minus infinity goes to 0.

In other words for numerical purposes we can say that as x goes to a large value why because numerically I cannot really go to infinity. I will put this slightly differently as L becomes large what is L, the L that we considered in the previous lecture psi goes to 0. Let me show this pictorially in the next slide.

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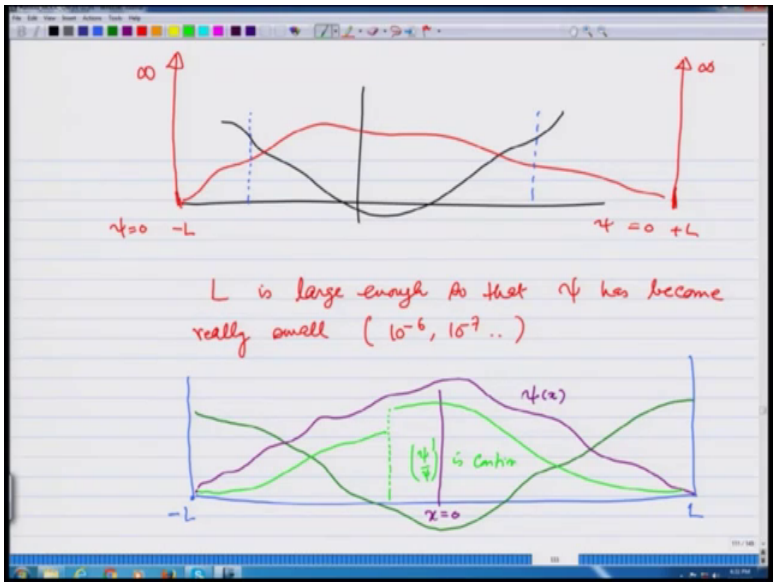

So, what we are considering is suppose there is a potential given the wave function is 0 far away. So, let us say psi is 0 and psi is 0 at these two points and then it does something in between. In essence what I am saying is I am putting infinite barrier here and whatever the potential does in between what I have to be careful about is that L, this is let us say minus L this is plus L, L is large enough. So, that psi has become really small. And what is that really small that is something that you have to decide maybe of the order of 10 raise to minus 6, 10 raise to minus 7 or so on. If you make L smaller and let us say in your numerical answer you made getting the numerical answer you have made L smaller.

From uncertainty principle I know that if I make L smaller the kinetic energy goes up. So, the energy eigen value out with getting would become slightly larger. So, when you do your integration to play around with your programme make L small and then start increasing it and you will see that the energy eigenvalue is coming down it is becoming smaller. So, now, with this introduction to integrate the Schrodinger equation becomes quite easy.

What I am going to do is in a sense what I have done is I have taken a large minus L, a large plus L. So, I have taken a huge infinite box and in between here is the potential no matter what the potential does and somewhere in the middle is my x equals 0. So, just like we did in the previous lecture I can start integrating form this psi, integrate my Schrodinger equation and make sure that the wave function goes t 0 to the other psi. Or

method two, I can start integrating from this psi I can start integrating from this psi and make sure that somewhere in the middle psi prime over psi is continuous.

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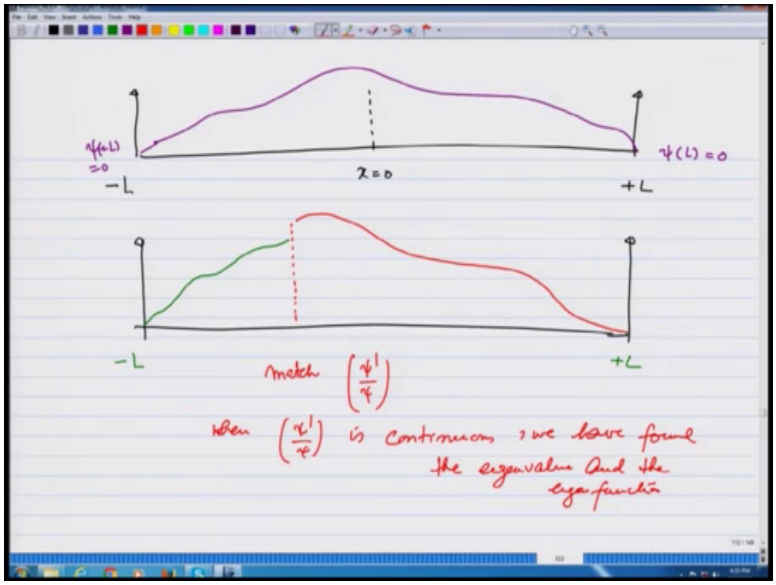

We are now going to enclose our system in a huge box this is x equals 0 and I have 2 methods one as I said I can start integrating from here starting with psi minus L equals 0 and come down to psi L going to 0 when they both become 0 you have found your eigenfunction. The other thing I can do is start integrating this is minus L plus L start integrating from here and somewhere in the middle start integrating from the right hand side and somewhere in the middle match psi prime over psi when psi prime over psi is continuous we have found the eigenvalue and the eigenfunction.

So, this is pretty much what solve in this one dimensional Schrodinger equation for general potentials is now there are some certain points and that is what I want to emphasize.

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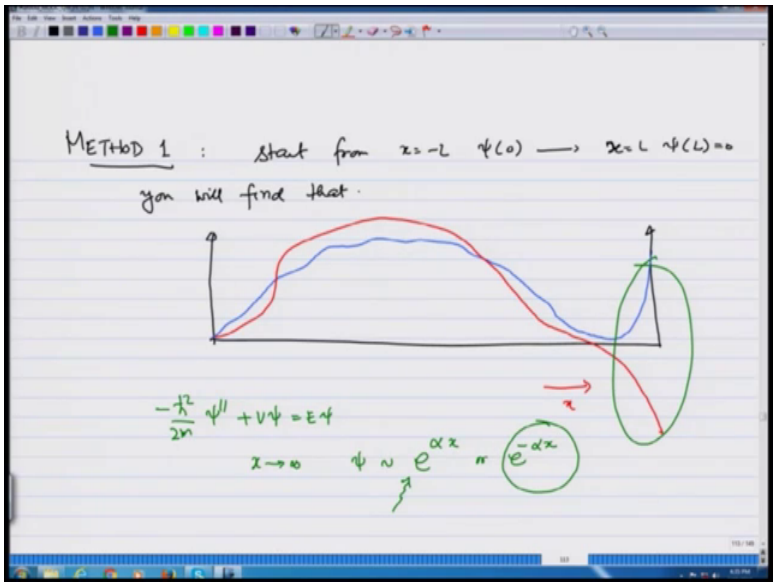

So, if I go by method one, which I said is start from x equals minus L psi equals 0 and go all the way up to x equals L and psi L equals 0 you will find that and now let me show this pictorially this is what happens the wave function would start from 0 to whatever it is supposed to do come down. So, that as if it is going to 0 and then it will start blowing up it could do this come down and then do this. So, what happens is as you go to large x a wave function rather than going to 0 even for the right eigenvalue it starts blowing up and there is a reason for it.

The reason is that from the Schrodinger equation psi double prime plus v psi equals E psi you find that x as x tends to infinity psi goes as E raise to some constant alpha x or E raise to minus alpha x. When we solve the problem by hand then we make sure that we pick this solution E raise to minus alpha x which is a decaying solution, when I solve it numerically there are always some errors peeping in and therefore, the second solution also it starts coming into the picture and as you go to larger and larger x it starts dominating the true solution which should go to 0. And therefore, you get this. To avoid this we always prefer to use the second method.

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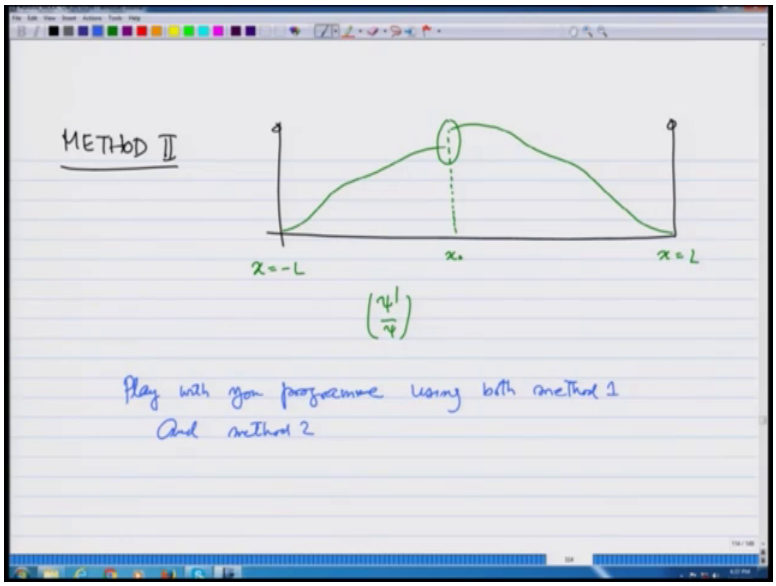

So, method two, which was that you start integrating from x equals minus L onwards you start integrating from x plus L coming back and then add some suitably chosen point x 0, it need not be 0 it need not be a prefix point you play around and see which is the best suited point and you match psi prime over psi why I said it is best suited point is a place where psi goes to 0 would not be a good point to choose a place where psi becomes very small would not be a good point to choose to match the boundary condition.

So, you choose a suitable point now for that you have to practice and you then match and then you get your answer. So, what I would urge you to do and the rest of the method is the same as in previous lecture that play with your programme using both method one and method two and see what you get more you practice better programmer better Schrodinger equation solver you would become. And you would always find that method two is gives you an answer where you do not have these problems of solution blooming up.

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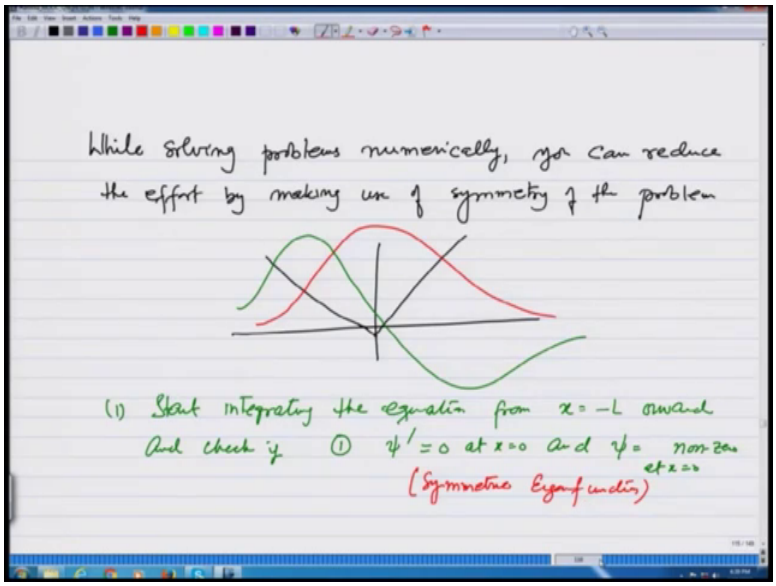

Now, you can always make use of the symmetry while solving problems numerically you can reduce the effort by making use of symmetry of the problem. So, by shifting the potential of something suppose I could make my potential symmetric about x equals 0. If it is not symmetric see if you shift it towards 0 and make it symmetric then I know that the solution is either symmetric or it is anti symmetric. So, what I can do in this case is start integrating the equation from x equals minus L onwards and check if number 1 psi prime is 0 at x equals 0 and psi is non zero at x equals 0 if that is the case you have found your eigenfunction and this would be symmetric eigenfunction.

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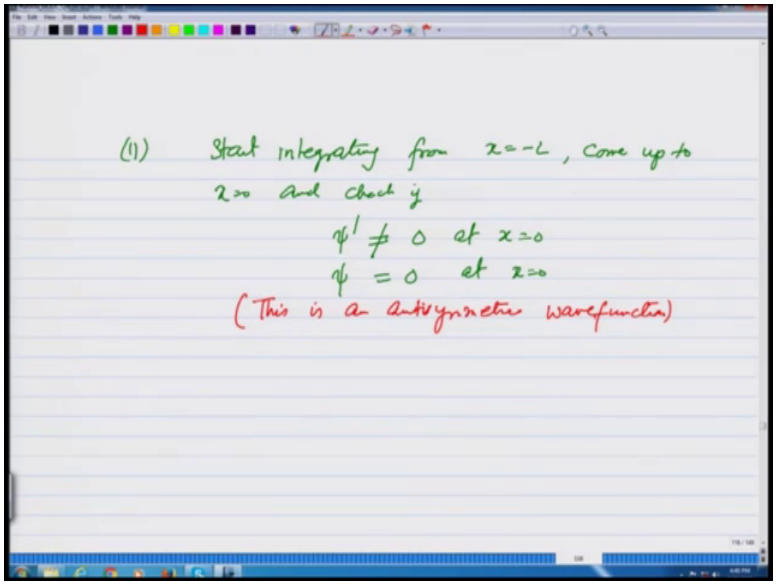

You can also check start integrating from x equals minus L from up to x equals 0 and check if psi prime is not equal to 0 at x equal to 0 and psi is 0 at x equals 0 then you have found anti symmetric wave function this is an anti symmetric wave function. So, in the case where the potential is symmetric you can make use of this symmetry of the wave function to integrate only half way and then pick up your wave function and then the other side is exactly either symmetric or anti symmetric with respect to whatever you have found.

So, what I would urge you to do now from now on is pick up a lot of problems, write your programs you may want to download your software you know the differential equation integrator form whatever is available on the net, but rest you have to do and you have to practice a lot that only makes you a very good programmer.

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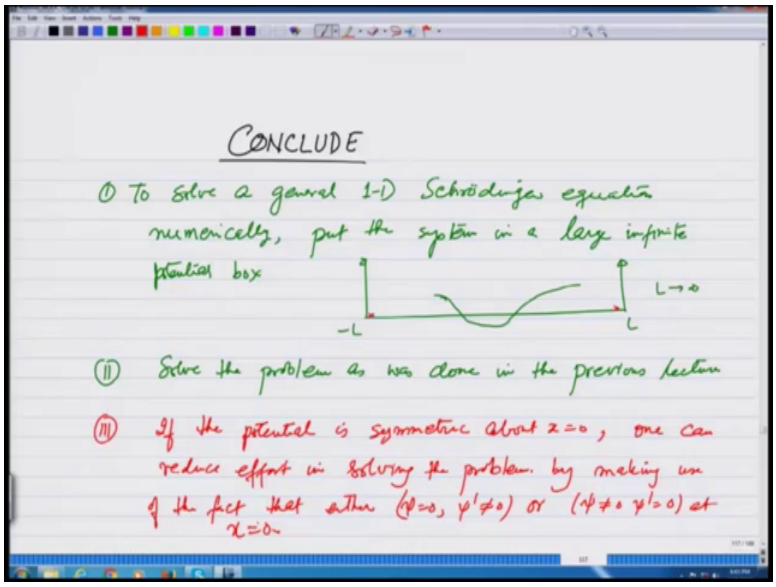

So, to conclude this lecture, to solve a general 1-D Schrodinger equation numerically put the system in large infinite potential box and by that you understand now that I am going to box which is huge minus L and L, L tending to infinity and system is somewhere here. So, that the wave function is effectively is becoming very small while the time you reach the boundary of this box and then solve the problem as was done in the previous lecture.

And third this is important if the potential is symmetric about x equals 0, one can reduce effort in solving the problem. By making use of the boundary condition at x equals 0 let me write that, by making use of the fact that either psi equals 0 psi prime not equal to 0

or psi not equal to 0 psi prime equal to 0 at x equals 0. That concludes the lecture on numerical solution of Schrodinger equation in one-dimension for a general potential.