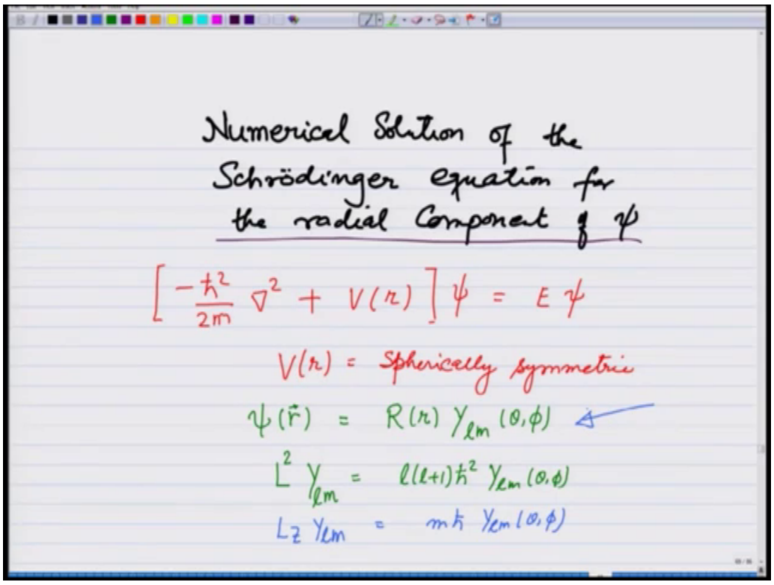
Introduction to Quantum Mechanics
Prof. Manoj Kumar Harbola
Department of Physics
Indian Institute of Technology, Kanpur

Lecture - 01
Numerical solution for the radial component of wavefunction for spherically symmetric potentials

During the last week I had introduced the Schrödinger equation for spherically symmetric systems, and discussed the properties of angular momentum and also the hydrogen atom and corresponding orbital's.

In this lecture I want to introduce you to the idea of solving the radial component of the wave function for a spherically symmetric systems, because not all potentials are such where analytical solutions are possible like they were for the hydrogen atom.

(Refer Slide Time: 00:54)



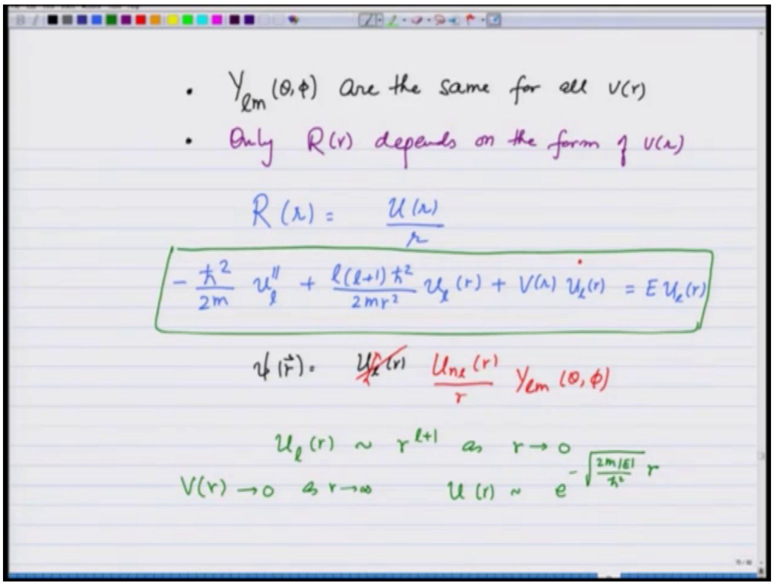
So, this lecture is going to be devour it to numerical solution of the Schrödinger equation for the radial component of psi.

So, you recall that the Schrödinger equation for 3 dimensional potentials was like this v as a function of only r, no vector which is for the spherically symmetric potential and this operating on psi give you e psi.

So, in this equation v r is spherically symmetric, and this is something that we have talked about in the previous lectures. And therefore, the wave function psi as a function of r vector can be decomposed through separation of variables as R r y lm theta. And phi where y l ms are the Eigen functions for the square of the angular momentum, y lm theta phi Eigen value being l, l plus 1 h cross square and also of the z component of the angular momentum which comes out to be m h cross y lm theta phi.

We discussed all this in the lectures last week what we want to focus on here is numerically on getting the solution of r.

(Refer Slide Time: 03:13)



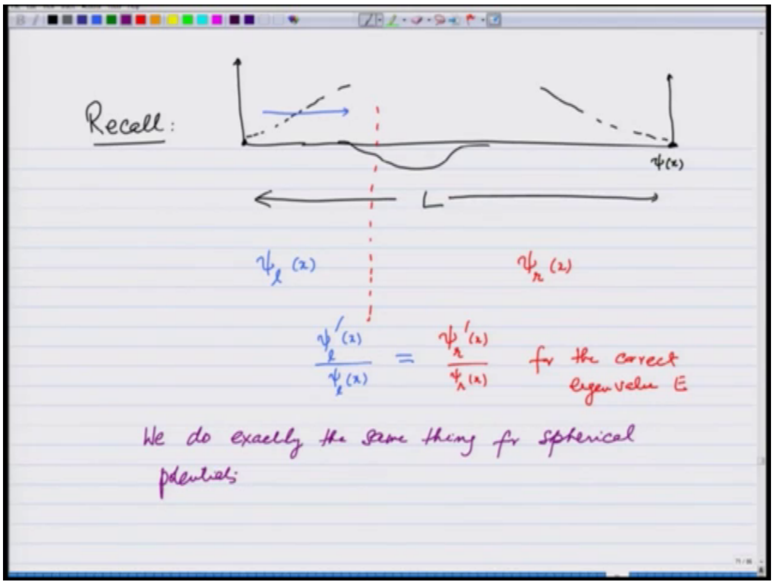
So, as you can see from the discussion So far y lm theta and phi are the same for all v r. And therefore, only R r depends on the form of v r, and last week we had solved for R r for very limited cases for the hydrogen atom potential.

Now, what we want to do now is solve this for a general v r, to facilitate the solution we had written R r as the function u r over r. So, that only the second derivative of u appears in the equation. And I will quickly write what the equation came out to be came out to be minus h cross square over 2 m, u double prime plus l plus 1 times l h cross square over 2 m r square u. And now I am going to write u l because this depends on l. R it is a function of only the radial coordinates plus v r u l r equals E u l r. This is a Schrödinger equation that we want to solve.

And then the wave function psi r is given as u l r let me also include n, n out here. So, I am going to write this as u n l r over r y lm theta and phi. So, focuses on u in this case. And we had derived some general properties and that was that for u l u l r goes as r raise to l plus 1 as r tends to 0. And for potentials that die off as r goes to infinity. So, v r that go to 0 as r goes to infinity, u r goes as e raise to minus square root of 2 m mod e over h cross square r, this we had derived.

So, what we want to do now is solve this numerically.

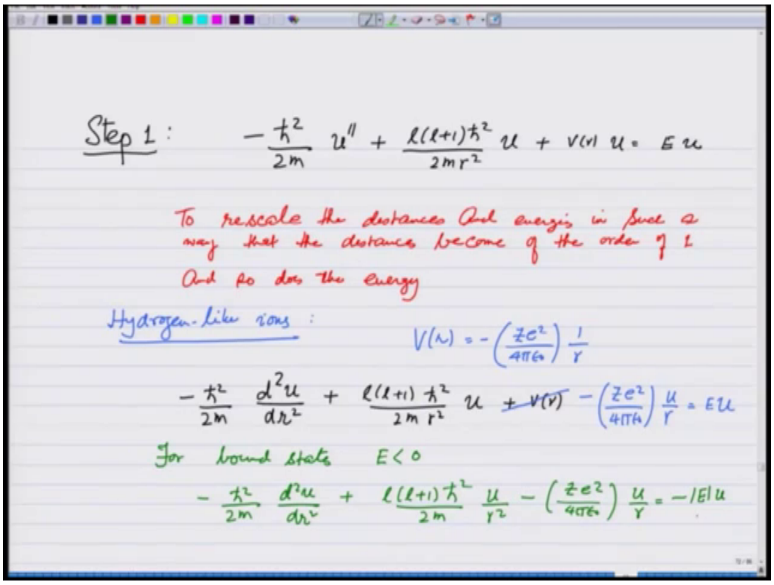
(Refer Slide Time: 05:59)



Recall the one dimensional cases, what we have done there for a general potential in x direction, we had taken a box which was a huge box of size l. So, the boundaries were really far off and taken the wave function psi x to be 0 at the boundaries, and then dealt up the solution from both sides. And then match the boundary condition in the middle.

What did we do in that case? We said let us take psi let me call the solution coming from the left side as psi left x. And we also calculate it psi right x. And in between at a point some x naught we said that we should have psi l prime x l means left here over psi l x should be equal to psi r prime x over psi r x for the correct Eigen value e. And that is how we build the solution. We are going to do exactly the same thing for spherical potentials. So, we do exactly the same thing for spherical potentials. So, let me take you through he numerical solution procedures step by step.

(Refer Slide Time: 07:59)



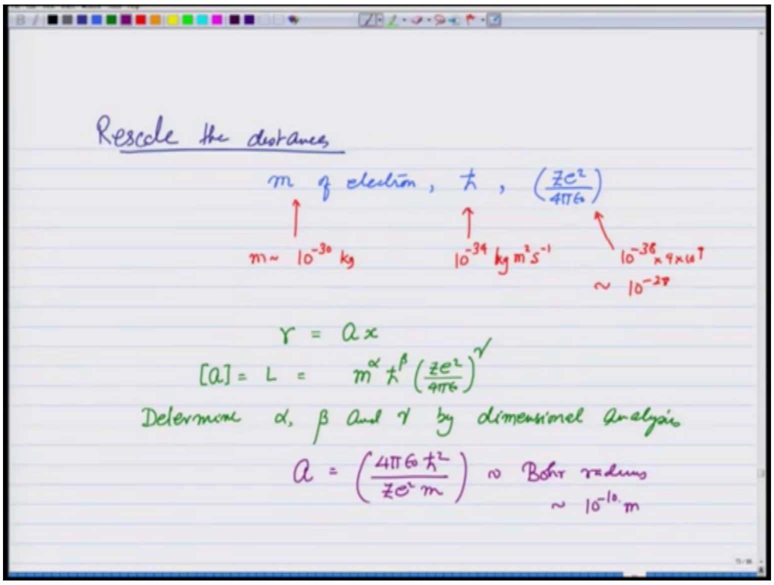
So step 1, I am solving the equation minus h Cross Square over 2 m u double prime plus l l plus 1 h cross square over 2 m r square u plus v r u equals e u. So, number one step one would be to rescale the distances and energies in such a way that the distances become of the order of 1. So, I am measuring r one 2 3 4 5 and so on. And so, does the energy.

I will illustrate this through an example. So, let us take the example of hydrogen atom or let me write hydrogen like atoms or ions; that means, v r is going to be of the form z e square over 4 pi epsilon 0, 1 over r with the minus sign in front. So, my equation for u is going to look like minus h cross square over 2 m let me write the double prime explicitly d 2 u over d r square plus l l plus 1 h cross square over 2 m r square u plus v r which are now I am going to replace by minus z e square over 4 pi epsilon 0, u over r equals u.

Now obviously, for bound states is going to be negative, e is less than 0. So, I am going to rewrite the equation as minus h cross square over 2 m, d 2 u over d r square, plus l l plus 1. H cross square over 2 m u over r square, minus z a square over 4 pi epsilon 0 u over r equals minus mod of e u.

Now, first thing I want to do is rescale the distances.

(Refer Slide Time: 11:01)



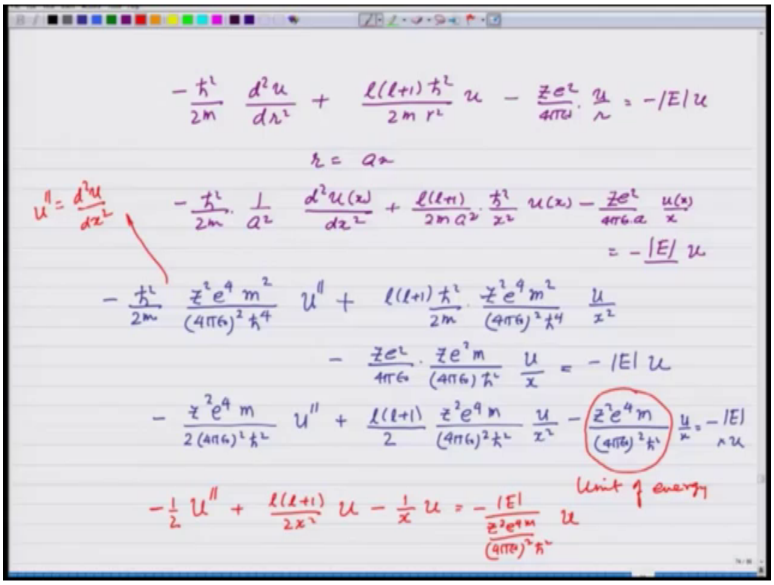
Now, here what do I have the parameters that are small in the whose terms I should write the distances. So, I have the mass of electron. I have the trans constant h bar, and I have z e square over 4 pi epsilon 0. These are the 3 external parameters that determine the problem.

Now, otherwise if I do not rescale you see the order of magnitude m as of the order of 10 raise to minus 30 kilograms, h is of the order of h processes of the order of 10 raise to power minus 34 k g meter square second inverse. And this quantity is of the order of 10 raise to minus 38 times 9 times 10 raise to 9. So, that is of the order of 10 raise to minus 28, these are very small quantities I cannot really take r to be in this order.

So, the way I rescale is I am going to write r is equal to some scaling factor a times x. And scaling factor a should be in terms of the mass h cross and z e square or 4 pi epsilon 0. So, let me write this a which has the dimensions of length in terms of mass of the electron raise to alpha, the trans constant raise to beta, and z e square over 4 pi epsilon 0 raise to gamma. And determine alpha, beta and gamma by dimensional. Analysis you do that and what you get is that a is going to be equal to 4 pi epsilon 0 h cross square over z e square m this is of the order of Bohr radius or 10 raise to minus 10 meters.

So now I am going to write r in terms of this a.

(Refer Slide Time: 13:56)



So, I have minus h cross square over 2 m d 2 u over d r square plus l l plus 1 h cross square over 2 m r square u minus z e square over 4 pi epsilon 0 u over r equals minus mod e u.

Let us write r equals a x. So, that this becomes minus h cross square over 2 m, 1 over a square d 2 u as a function of x over d x square plus l, l plus 1 over 2 m a square h cross square over x square u x, minus z e square over 4 pi epsilon 0 a u x over x equals minus e over nothing over times u minus e times u.

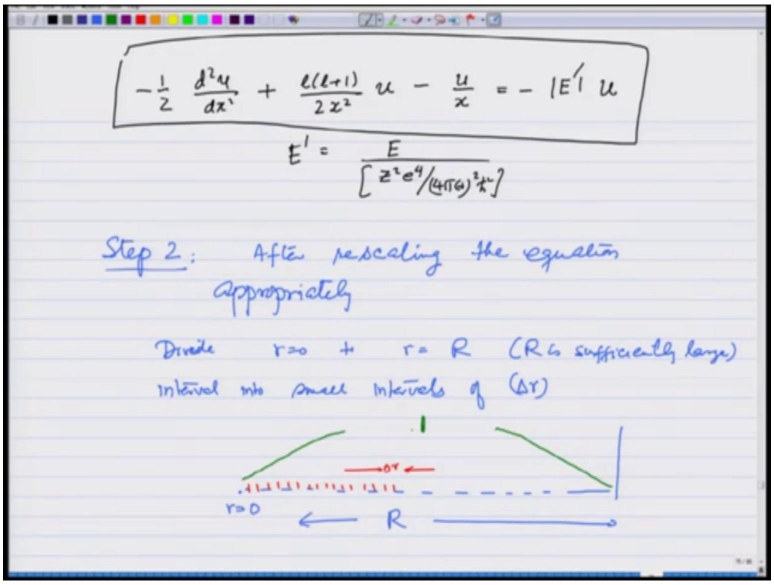
Now, substitute the value of a. So, you get minus h cross square over 2 m z, square e raise to 4 m square over 4 pi epsilon 0 square h cross raise to 4, u double prime where u double prime let me write it here u double prime now indicates d 2 u over d x square, plus l l plus 1 h cross square over 2 m again z square e raise to 4 m square over 4 pi epsilon 0 square h cross raise to 4, u over x square minus z e square over 4 pi epsilon 0 1 over a is going to be z e square m over 4 pi epsilon 0 h cross square, u over x is equal to minus mod e u.

You simplify all this and you get minus z square e raise to 4 m over 2 4 pi epsilon 0 square h cross square u double prime plus l l plus 1 over 2 z square e raise to 4 m over 4 pi epsilon 0 square h cross square u over x square minus z square e raise to 4 m over 4 pi epsilon 0 square h cross square u over x equals minus mod e times u.

Notice that naturally this quantity which I am encircling by red is unit of energy you can easily check that. Because this is nothing but z square e square over 4 pi epsilon naught a, which is nothing but the electrostatic energy if 2 charges are at a distance a. So, this is a natural unit of energy.

So, you take it to the other side and you get u double prime minus a half u double prime, plus l l plus 1 over 2 x square u minus 1 over x u equals minus mod e over z square e raise to 4 m divided by 4 pi epsilon 0 square h cross square u, that is the equation.

(Refer Slide Time: 18:24)

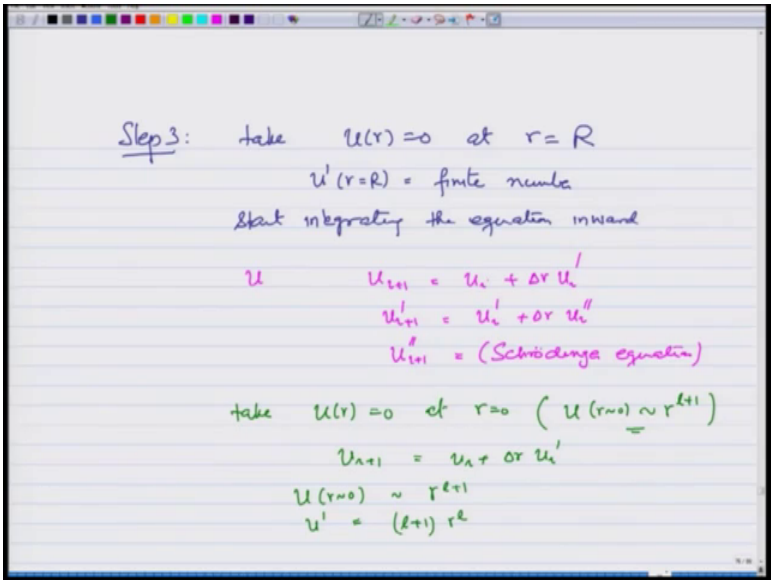


So, the equation you get finally, looks like minus 1 half d 2 u over d x square plus l l plus 1 over 2 x square u, minus u over x is equal to minus this rescaled let me call this energy e prime u where e prime is nothing but e divided by z square e raise to 4 divided by 4 pi epsilon 0 square h cross square. Now you see this equation looks very simple all these constants have been taken into the units of distance and energy.

Step 2 after rescaling the equation appropriately, I gave you the example of rescaling the hydrogen atom equation. They could be some other equations where you have to rescale slightly differently. So, appropriately whatever rescale you do, now divide r equal to 0 to some r equals r, where r is sufficiently large. Divide this interval into small intervals of some delta r right.

So, what we are doing is here is my r equals 0, and I am taking a large distance out where wave function is supposed to vanish. Because this distances r and I am dividing this whole thing in towards called a mesh of small delta r intervals to integrate the equation. So, each of this interval is delta r and what I will do like the equation for one dimensional systems essentially a one dimensional like system, I will start integrating from r equals 0 onwards start integrating from r equals capital r inwards and somewhere in between I will match the solution.

(Refer Slide Time: 20:51)

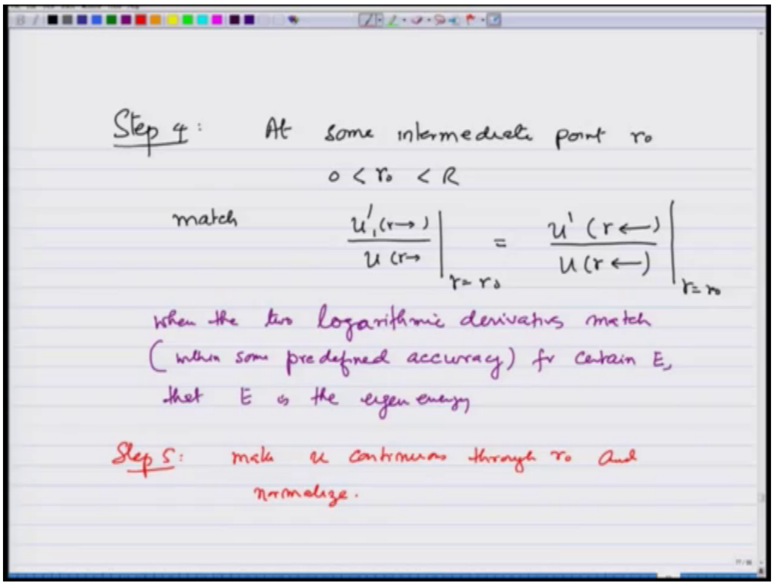


So, what do I do now step 3? Take u r to be 0 at r equals r and that is why it is important that capital r be very large where wave function essentially vanishes. And take u prime r equals r to be some finite number and start integrating the equation inward. I have told you how to integrate the equation in the case of one dimensional potential. So, you may have to go back and see how it is done.

So, essentially what you do is you take a u and take u i plus 1 to be equal to u i plus or minus depending on whether you are integrating in or integrating out delta r times u y prime u y prime. You again update by delta r u I double prime and you now update this is i plus 1 u i plus 1 double prime you update through the Schrödinger equation, because this depends on the value of u at that point. So, you start integrating inward and you also take u r to be 0 at r equals 0 because recall that u near r equals 0 goes as r raise to l plus 1.

So, even for l equals 0 it is 0 and you start integrating out. So, again you do u i plus 1 equals u i plus delta r times u i prime. Now here since you know the behaviour you can take some help from there u at r equals 0 goes as r raise to l plus 1. So, you can also write u prime equals l plus 1 r raise to l and you start building up your solution from first and second point onwards.

(Refer Slide Time: 23:09)



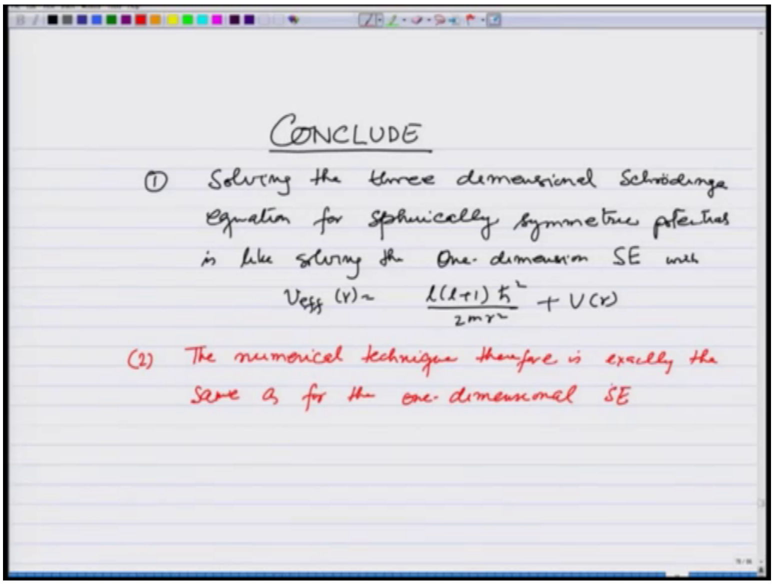
And then step 4 at some intermediate point r naught. So, r naught is greater than 0 less than r match u prime coming from r out divided by u r out at r equals r naught, 2 u prime r coming in divided by u r coming in. So, they have to indicate 2 different solutions your developing at r equals r naught.

When the 2 logarithmic derivatives match, and I have to say it within some predefined accuracy. We never get into match perfectly you can say the match within 10 raise to 3 10 raise to minus 4 10 raise to minus 3 or So on for certain E. That E is the Eigen energy. So, you found your Eigen energy then you rescale and again normalize the wave function and all that.

Now, I have given you steps to do this you will have to practice it yourself. I cannot do more than this and the best way to learn it is to practice it yourself. Take whatever help you have from available softwares whatever language you know, but try to make this mesh yourself. Try to write the integrating software yourself and solve it and then after this step 5; obviously, yes then step 5 make u continuous through r naught; that means, you match them again and normalize. And that gives you the solution of the problem.

You scan over E start from a very largely negative energy and you start scanning and you will find solutions for different energies. Many, many Eigen energies, many, many Eigen functions and then you order them according to the energy Eigen values you are getting. So, this is for you to practice and learn beyond this there is not really much to do in numerical integration of Schrödinger equation.

(Refer Slide Time: 26:12)



So, to conclude this lecture solving the 3 dimensional Schrödinger equation for spherically symmetric potentials, is like solving the one dimensional Schrödinger equation with v effective r equals l l plus 1 h cross square over 2 m r square plus the v r that is given. And then the technique the numerical technique therefore, is exactly the same as for the 1 dimensional Schrödinger equation that is what I have discussed in this lecture.

So, this concludes basically our discussion of solution of the Schrödinger equation for spherically symmetric potentials from next lecture onwards, I am going to concentrate on another system which is free electron light. But now we will have periodic potentials there, and therefore that solution differs slightly from the free electron solutions and gives rise to bands.