Basic Quantum Mechanics

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Module No. # 04

Simple Applications of Schrodinger Equation

Lecture No. # 2

The One Dimensional Potential Well and Particle in a Box

In my previous lecture, near the end of the previous lecture, we had started with the solution of the particle, in a one-dimensional potential. Well, we will continue with that, and we hope today we will be able to start the solution corresponding to a particle, in a three dimensional box, which has many important applications.

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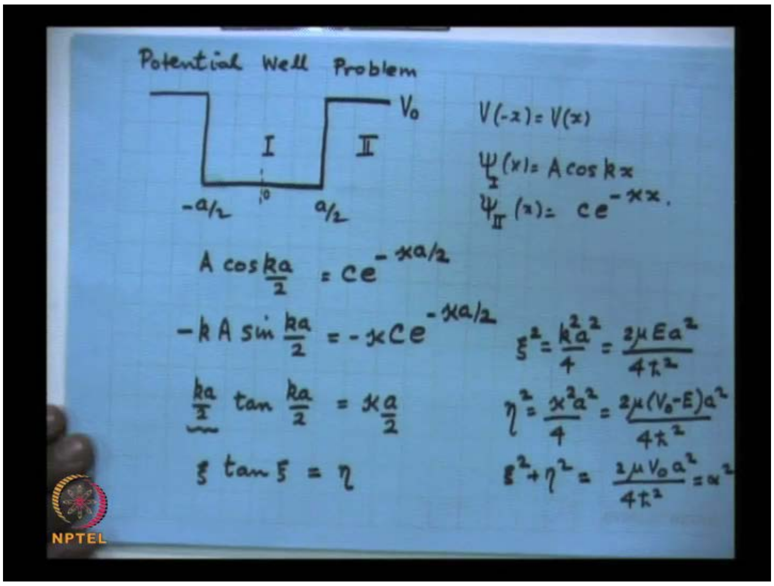

So, let us start with the one dimensional potential well problem, in which the potential is 0, between x less than a by 2 and lying between minus a by 2 and plus a by 2 and V 0 outside. So, the particle is confined, in this well. And, we had solved the Schrödinger equation; this is the origin, since V of minus x is equal to V of x the potentially symmetric. So, the wave functions, are either symmetric or anti symmetric.

First, we considered the symmetric wave function and we solved it and we found that the solution of the Schrödinger equation in region one, was equal to a cos k x and the solution in the second region was equal to c into e to the power of minus kappa x. So, you have here, an exponentially decaying solution in the second region. We then match the wave function at, x equal to a by 2 and it is derivative. So, we got two equations, a cos k a by 2, is equal to c into e to the power of minus kappa a by 2, this is the continuity of wave function at x equal to a by 2.

And the continuity of the derivative, will be the differential minus sin k a by two is equal to minus kappa c e to the power of minus kappa a by 2. And, if I divide for non-trivial solution as we discussed last time, one with respect to the other.

We will have k a by 2 tan k a by 2 is equal to kappa a by 2. We write this quantity as xi. So, xi tan xi is equal to eta, where eta is equal to kappa a by 2. So, we know that xi square is equal to k square a square by four or this is equal to two mu e a square by four h cross square and eta square is equal to kappa square a square by four. So, kappa square is equal to 2 mu V 0 minus e a square by four h cross square and xi square plus eta square. If, I add these two equations as we did last time. So, the e will cancel out. So, we get 2 mu V 0 a square by four h cross square, which is a constant. So, this I put as alpha square.

So, then eta square is equal to alpha square minus xi square. And, therefore, eta will be equal to alpha square minus xi square. So, you see for a given value of mu, for a given value of a and of course, h cross is a constant, the only unknown parameter is xi e and therefore, xi. For a given potential well, alpha is known, mu is known, V 0 is known, a is known, h cross is a constant. So, alpha is a number, may be, we will discuss a very simple example little later.

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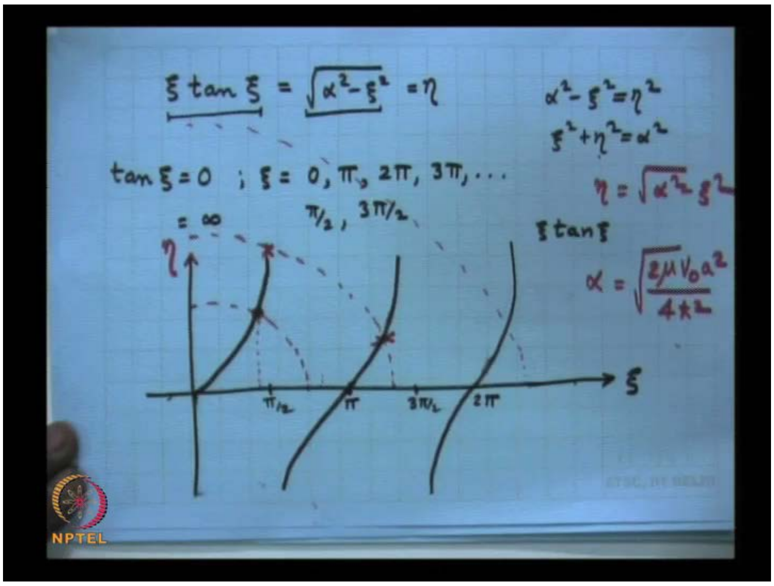

Therefore, the transcendental equation is, xi tan xi for symmetric states is equal to alpha square minus xi square, we said both of them equal to eta. So, what we do is that, we plot the left hand side and the right hand side, as a function of xi. Now, what is the right hand side? So, as we have seen that if I square this, I get Alpha Square minus xi square is equal to eta square. So, xi square plus eta square is equal to alpha square. So, in the xi eta plane, x square plus y square is equal to alpha square is the equation of a circle of radius alpha.

Now, the left hand side as you know that, tan xi is equal to 0, for xi is equal to 0, pi 2 pi and 3 pi and tan xi is equal to plus or minus infinity at pi by 2, 3 pi by 2 and so on. So, let me plot this carefully. So, I have here the horizontal axis is xi. So, as xi equal to 0, it is zero and it will go to infinity, at pi by two and then there is a discontinuity like this. And, then it will become infinity like this, because tan xi has an infinite discontinuity at pi by two and it will become zero at pi, then it will become infinity at 3 pi by two and so on.

So, this is the plot of xi tan xi, as a function of xi, it will have infinities at pi by 2, 3 pi by 2, 5 pi by 2 and so on. And, if you have zeroes at 0 pi, 2 pi and 3 pi, now this is the left hand side, let me now plot the right hand side. Right hand side is the eta axis. So, eta square is equal to under root of alpha square minus xi square. So, this is quadrant of a circle. So, I will ask you, to tell me the value of alpha, if alpha is 2, then I will draw a quadrant of a circle, this is pi by 2 that is 1.5. So, 2 is somewhere here and if alpha is 2 I will have a circle of radius 2. Then at this point, the left hand side and right hand side are equal. And, the value of xi, that is suppose something like 1.4 or something, that is a Eigen state of the problem.

So, what is alpha? Alpha is under root of 2 mu V 0 a square by 4 h cross square, if suppose, alpha is four, then I have to draw a circle of radius four unit. So, pi is here, 3 pi by 2 is here, 4 will be somewhere here. So, I will draw a quadrant of a circle, of radius 4 and then there will be two places where the left hand side will intersect, the right hand side. And, there will be then two symmetric states, we have considered till now only the symmetric states.

We will consider the anti symmetric stages in a moment. So, these are the discreet Eigen values of the problem and whenever you have an equation like this, you say it is a transcendental equation; it is satisfied only, when the left hand side is equal to the right hand side. And that will happen only for certain discrete values of xi. If, xi was equal to eight, then you have to draw a circle of radius eight, if alpha is eight, then you'll have three symmetric notes.

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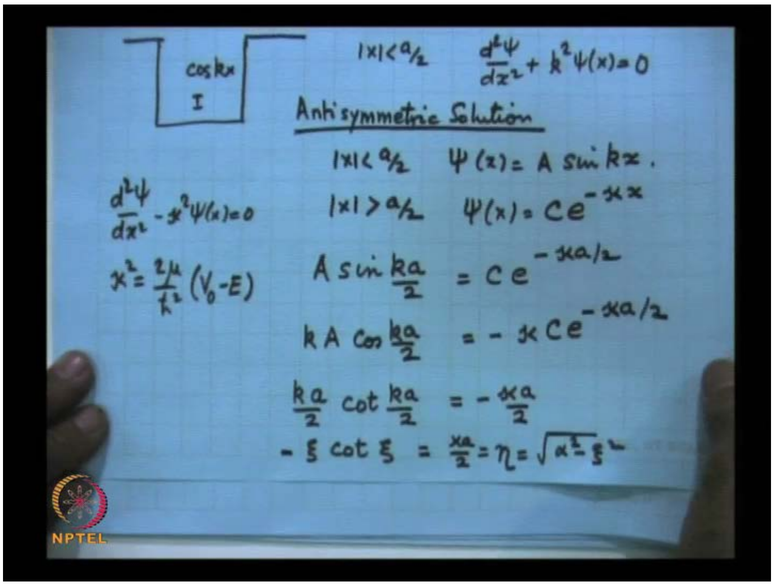

Let me skip here, for a moment, we will come back to this figure a little later. Now, consider the anti symmetric stage. So, we will go back to the potential well, that we had discussed earlier, that I have here this, as the potential well, till now we have considered, the symmetric states, in which the solution is cos k s in this region.

So, region one is x less than a by 2, the Schrödinger equation is d 2 psi by d x square, plus k square psi of x is equal to 0. So, solution can be either, cos k x or sin k x. So, now we consider the anti symmetric solution. In the anti symmetric solution, we will have in the region x less than a by 2, we will have psi of x is equal to a sin k x and for x greater than a by 2, we will have again the same solution.

The Schrödinger equation will be d 2 psi by d x square minus kappa square psi of x is equal to 0. So, the solutions will be psi of x will be an exponentially decaying solution, minus kappa x. once again, we apply the continuity conditions. The continuity of the wave function will be, a sin k a by 2, will be equal to c e to the power of minus kappa a by 2 and x is equal to a by 2 psi of x should be continuous.

And then, I have the derivative continuous, that is, k a cos k a by 2 is equal to minus kappa c e to the power of minus kappa a by two. So, I again divide this equation and a cancels out. So, non-trivial solution, I multiply k a by 2 cot k a by 2 is now equal to minus kappa times a by 2. The value of kappa is still the same, which is equal to 2 mu by h cross square V 0 minus e. So, once again, I will have the similar kind of thing. So, I take the minus sign here. So, I get minus xi cot xi is equal to kappa a by 2, that is eta and that we have shown to be, equal to the under root of alpha square, minus xi square.

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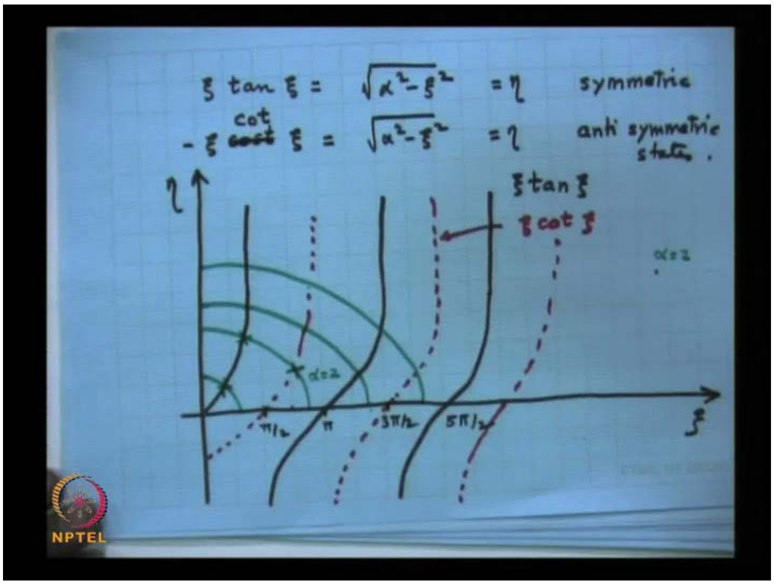

So, the right hand side remains the same. So, we summarize the result. So, for the symmetric solution we had xi tan xi is equal to under root of alpha square minus xi square and minus xi co tangent of xi is equal to under root of alpha square minus xi square.

So, this is equal to eta, and this is equal to this corresponds to symmetric states and this corresponds to ant symmetric states. Now, let me plot it again. So, we will have something like this, suppose this is pi by 2, this is pi, this is 3 pi by 2 and so on. So, xi tan xi goes to infinity here, So, you have pi by 2, 3 pi by 2 and 5 pi by 2 and this will go to infinity, what I have plotted, is xi tan xi, as a function of xi. So, this is eta, now let me plot minus in red pen. So, co tangent xi times, co tangent xi tends to a finite number at xi equal to 0, because cot xi tends to infinity, xi tends to 0 so, the product is, pi by 2 cot xi is 0.

So, it will go to infinity at pi and then it will go like this, at pi 5 by 2 it will go to infinity. So, the quantity which I've shown, with red pen is xi cot xi. And, there will be again at 5 pi by 2 this, at this point will be infinity. In the right hand side, is a quadrant of a circle, whose radius is alpha. So, let me say alpha is equal to 2. The quantity 2 is less than pi. So, the quadrant of the circle would be something like this is pi by 2. So, you can see that, there'll be one symmetric and one anti symmetric state.

If alpha was equal to 1, then this will be only one symmetric state, only one discreet state. If alpha was 4, then this is the radius which is greater than pi, then there will be two symmetric states and one anti symmetric state. And suppose alpha is 6, then you'll have to draw a radius of 6 then, it will be two symmetric states and two anti symmetric states. As, the value of alpha becomes larger and larger, that is as the value of the 0 becomes larger and larger, we will have larger and larger number of discreet states, that are possible.

In general, a potential well has a finite number of states; it has a finite number of discreet states. And, how to determine the number, when you given the value of mu, given the value of V 0, given the value of a and I know h cross, I will first calculate the value of alpha. If the value of alpha is less than pi by 2, I know that there is one symmetric state. If alpha lies between pi by 2 and pi then, one symmetric and one anti symmetric. If alpha lies between pi and 3 pi by 2 then two symmetric and one anti symmetric and so on.

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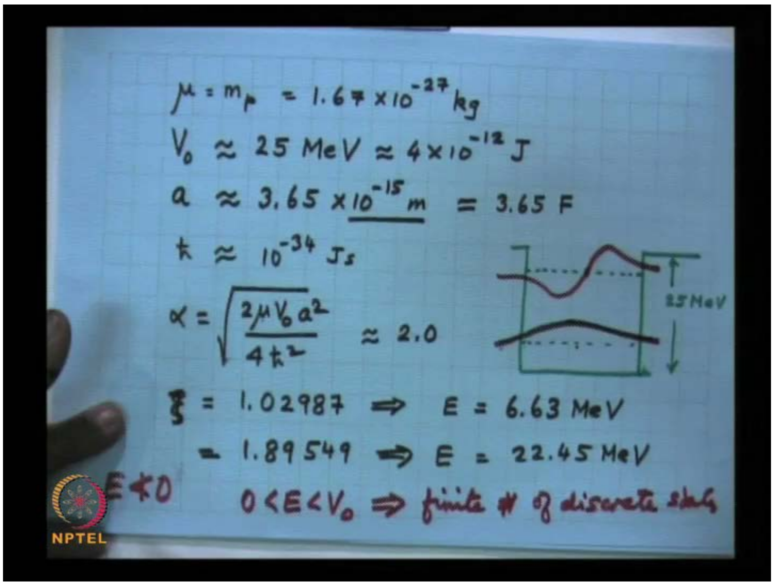

So, let me consider a simple case, a proton in a potential. So, I assume that the mass of the particle, is the proton mass and the proton mass is about 1.67 into 10 to the power of minus 27 k g. suppose, this approximately represent the deuteron problem 25 M e V. So, this is about 4 into 10 to the power minus 12 joules, 25 M e V and a the range of the potential is equal to 3.65 into 10 to the power of minus 15 meters is known as a Fermi, in honor of the famous nuclear physicist, Enrico Fermi, 3.65 Fermi. One Fermi is 10 to the power minus 15 meter.

And you know the value of h cross, which is about 10 to the power of minus 34 joule. It is always better to use, consistently the m k system of unit, and then there is no chance of an error. So, if you substitute, this is equal to 2 mu V 0 a square by 4 h cross square, you substitute for mu, 1.67 V 0 is 10 to the power minus 7 joules, a is 3.65 into 10 to the power minus 15 h cross is 10 to the power minus 34, if you substitute that and take the under root you will get alpha is equal to 2.0.

So, if alpha is 2.0. So, then alpha lies between pi by 2 and pi. And, therefore there will be two symmetric states. So, there are two states, one symmetric and one anti symmetric, the corresponding values of xi, for which the left hand side is equal to the right hand side, this is equal to 1.02987 it can be obtained very easily. And the corresponding value of e comes out to be 6.63 M e V and the other value is 1.89549, the corresponding value of e is 22.45 M e V. Suppose, if alpha is equal to 2. So, this is the first value of xi and this is the second value of xi, these are the discreet energy Eigen values of the problem.

So, therefore we obtained two states and for this particular problem, the potential well and the ground state, that is the depth is about 25 M e V and here is the first state which has 6.63. And, the wave function will be a symmetric wave function like this.

It should be cosine solution here and exponentially decaying solution here. And the second one which is right at top has a value of about 22.45 M e V and it will be an ant symmetric solution.

So, it will be zero here and something like this. This is the symmetric solution cosine insigne and outside it is exponential this is an anti symmetric solution. We showed that in the harmonic oscillator problem, there were alternately symmetric and anti symmetric. First, the ground state is symmetric then anti symmetric then symmetric then ant symmetric and so on. This same is true in all cases that you'll have first the symmetric state then ant symmetric and in this particular case there are only two discreet states.

There are, only finite number of discreet states if it were instead of two twenty five M e V if it were 200 and 50 M e V then there would have been a much larger number of states so, finite number of discreet states. I would like to conclude this discussion by mentioning that we have considered only zero less than e less than V 0.

And we have obtained we have shown that we will have a finite number of discreet states. E can never be less than zero, because no condition can be satisfied e can never can be less than 0 then the minimum value of the potential energy e can of course, be greater than 0 e can of course, be greater than 0 then once again you'll have a particle which comes in from the left and will get reflected and will get transmitted.

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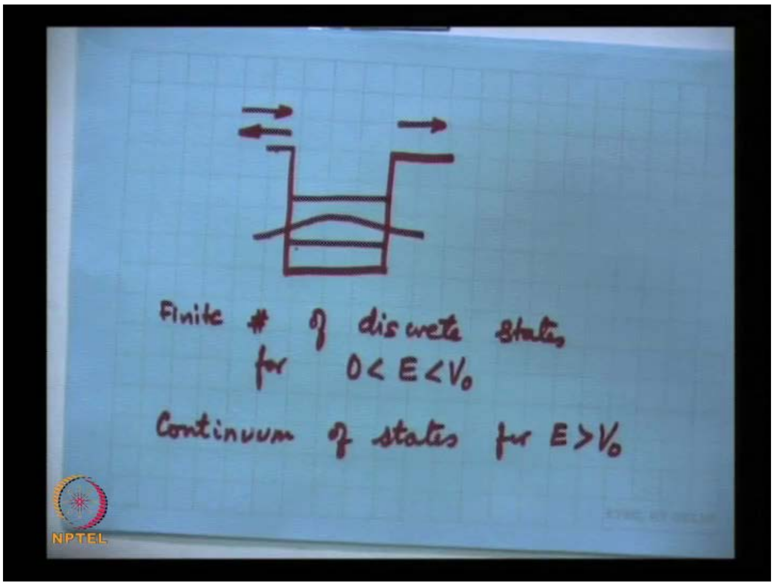

So, therefore, in this particular case what I told you at the end is important, that you have two states two types of solution one discreet bound state in which the wave function is exponentially decaying at large distance and then you have incident wave and the reflective wave. So, you have a finite number of discreet states discreet states for E lying between 0 and V 0.

And the continuum of state that is all possible values of an for e greater than V 0. These are also known as scattering states. In all problems of quantum mechanics for a given potential energy distribution you have two types of solutions one is the discreet bound state solution and the other is the continuum of scattering state solution.

And the simplest example that I could think of is the simplest atom hydrogen atom. We will discuss that in greater detail later, but the hydrogen atom you know it consist of a proton and an electron and there are two types of solutions.

One in which the electron and the proton are together to form a bound state and you have discreet energy level of the atom. These are, the discreet bound state of the Schrödinger equation and the second is let us suppose, proton is here and the electrons is coming from the last distance.

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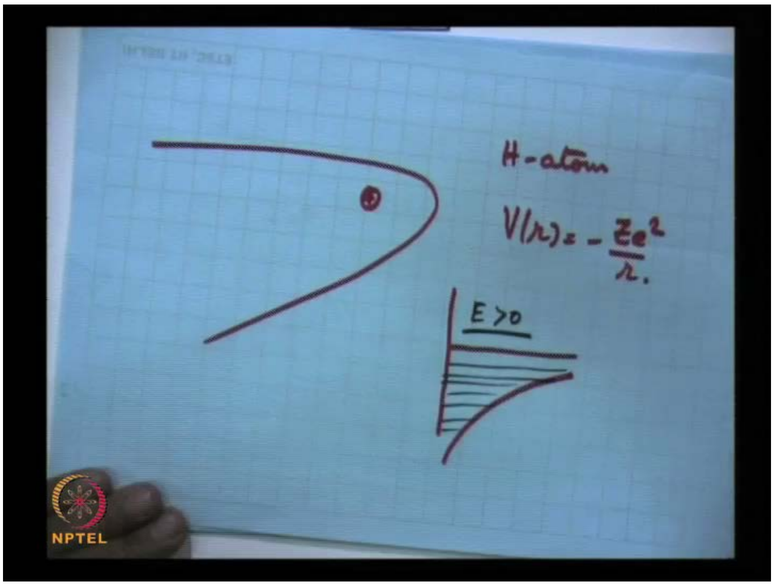

Proton is coming here and the electron is coming and getting scattered. Here, it is a continuum of energy value all possible values of energy are allowed. And these are the scattering states. So, in the hydrogen atom problem in the hydrogen atom problem you will have the potential energy function is given by minus z e square by r and if you plot this z e square by r minus z e square by r then you'll have a set of discreet state in fact, infinite number of discreet states.

These are the lead to the hydrogen atom spectrum and for e greater than zero you'll have a continuum of states in which a particle will come from last distance interact with the proton and gets scattered that hopefully we will discuss at a later time.

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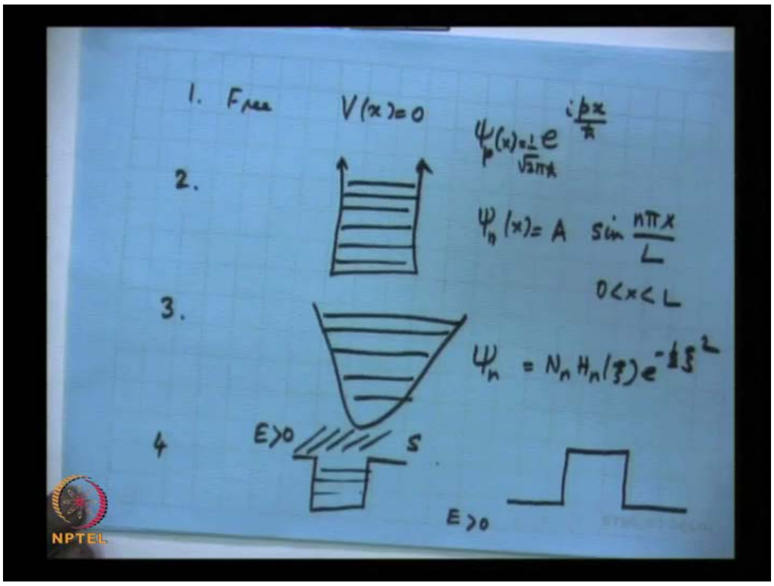

So, till now we have considered four five problems. First we consider the free particle problem in which the potential energy is zero everywhere. We found only plane wave solution continuum of wave function and we found this was i p x by h cross these are the wave functions psi p of x. All values of energy are allowed you normalizes by putting one over root two pi h cross then you, consider a particle in an infinitely deep potential box that, this is infinite then you have only discreet states no continuum of states.

Only, discreet states and we had psi n of x, which is equal to the normalization constant sine n oi x by l and you have a this from 0 less than x less than l then. We consider the harmonic oscillator problem in which there is V of x is half mu.

This also has an infinite number of discreet states. The wave functions are as I have told you many times these are the hermit gauss functions. Finally, we consider that potential well problem and in which there are two classes of solutions. One discreet bound states finite number of discreet bound states and for e greater than zero you have a continuum of states. These are the scattering states and when we consider this problem then there are no bound states only all values of E greater than 0 are allowed. These are a continuum of scattering states.

So, if you solve the Schrödinger equation for a given potential distribution. We have considered consistently only one dimensional potential problem. Then, you will get two types of solutions. One in which the particles are confined at the origin, those are the discreet bound states for the problem and the energy levels are discreet and then you have in addition a continuum of scattering states which may or may not exist.

For example in the case of the harmonic oscillator problem or in the case of a particle in an infinity deep potential well problem there are no scattering states. So, this almost completes this analysis of one dimensional problem. Today, I want to continue the discussion and consider a very simple and very important problem of particle in a box and it very accurately represents the free electrons in a metal.

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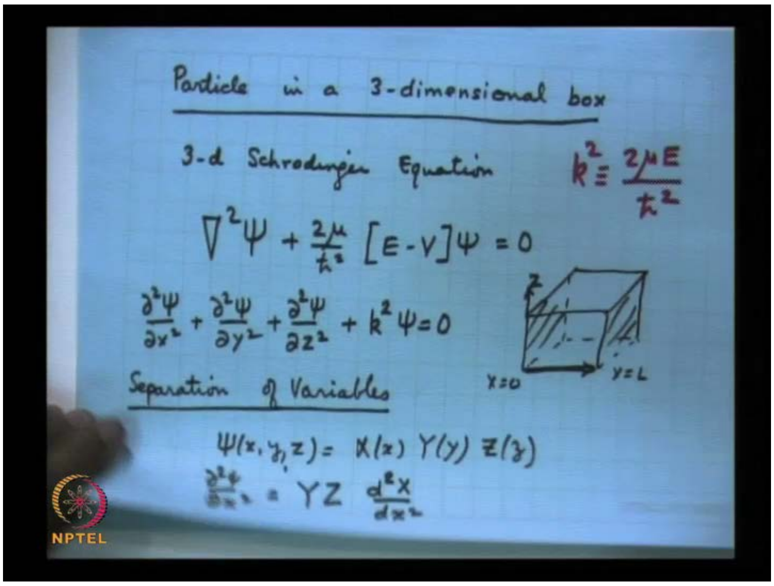

So, we do the particle in a three-dimensional box in a three dimensional box. And of course, we have to solve the three dimensional Schrödinger equation. This is the probably simplest and a very important solution of the Schrödinger equation.

So, the three-dimensional Schrödinger equation is given by del square of psi plus two mu by h cross square E minus v psi of x y z is equal to 0. Now I consider an electron or a proton which is confined inside a box, whose side is l that is what I mean by confined it is an infinitely deep. But it is a three-dimensional box the particle cannot go out of the box and therefore, the wave function has to vanish, at all point of the surface of the box. So, for example, if I take this as my x axis so, this plane is x equal to 0 and this plane this side is x equal to l and similarly, if the vertical axis is the z axis then the base is z equal to 0 and the top one the top roof is z equal to l.

And of course, for a problem like this, one has to use Cartesian system of co ordinates and therefore, the del square psi operator becomes delta two psi by delta x's square plus delta 2 psi by delta y square, plus delta 2 psi by delta z square. And inside the box the potential is zero. So, therefore, V is 0. So, you get 2 mu e by h cross square psi. So, that I represent by k square psi is equal to 0. Where, k square let me write it down by red. K square is defined to be equal to once again two mu e by h cross's square I want to solve this problem. So, once again I have a box of length I have a metal for example, I have a metal cube each side is of length l.

There is an electron free inside the metal, but the potential is so, deep that it cannot escape from the metal. So, the wave function associated with the electron must vanish on the surface of the metal. So, let me solve this equation and apply the boundary condition that on all six faces the wave function is zero. So, we use the method of separation of variables. So, this is the method of separation of variables.

And we write this as psi of x y z as equal to x of x y of y and z of z let me try the sum this is the method which sometimes it works sometimes it does not work, but in this case we know that it will work therefore, we are using that. So, what is delta two psi by delta x square. So, this will be delta two psi by delta x square will be equal to this and this will be constant. So, y and z can be and then become the differential d 2 x by d x square.

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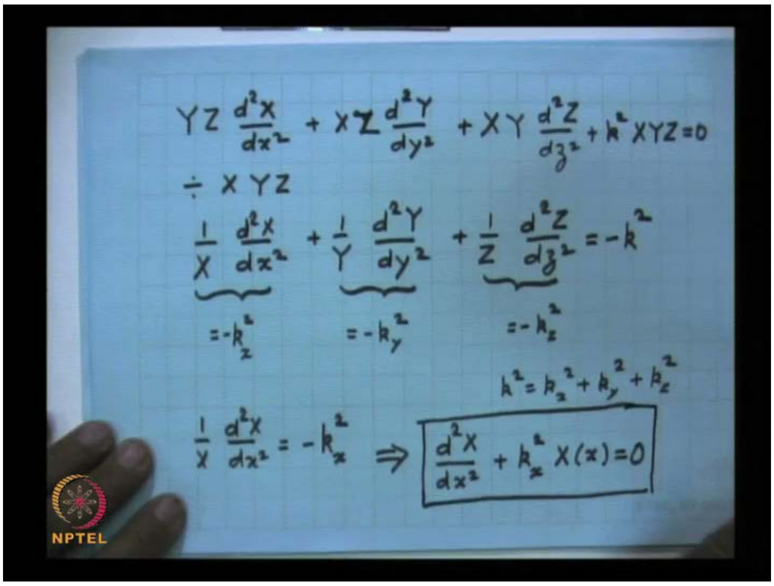

And similarly, delta 2 psi by delta y square and delta 2 psi by delta z square; so, if I substitute the solution with this equation; then what I will get is the following d sorry y times z into d 2 x by d x square remember that we have assumed that let me do this again let me do this again. We have assumed that psi of x is equal to x y x y and z. So, we substitute it in this equation. So, we get y z d 2 x by d x square then x y d 2 x z d 2 y by d y square plus x. The third term will be x y d 2 z by d z square plus k square into psi is x y z. X as a function of x y as a function of y and z as a function of z. So, I substituted this solution in this equation and I obtain this. The next is very simple that, I divide the whole equation by psi that is I divide by x y z. So, I get one over capital x d 2 x it is a very straight forward d 2 x by d x square plus one over y d 2 y by d y square plus 1 over z d 2 z by d z square plus k square and k square. So, this I write as minus k square now this is a function of x this term is a function of y and this term is a function of z.

How can a function of x and plus a function of y and plus a function of z be equal to a constant. You know x y z are independent variables it could only happen if each term is a constant. So, I this must be equal to, let us suppose minus k x square. You cannot set it equal to your positive constant, because then as we will show later it will not be able to satisfy the boundary conditions. This will be equal to minus k y square and this will be equal to minus k z square.

Then you will have k square is equal to k x square plus k y square plus k z square k x k y k z are just are numbers symbols. So, one over x d two x by d x square I have said this equal to your minus of cos v, as I have said this equal to k x square. So, therefore, if I multiply this out this will become d two x by d x square plus k x square multiplied by x of x is equal to 0 now obvious equation this is a simple second order equation and I know the solution.

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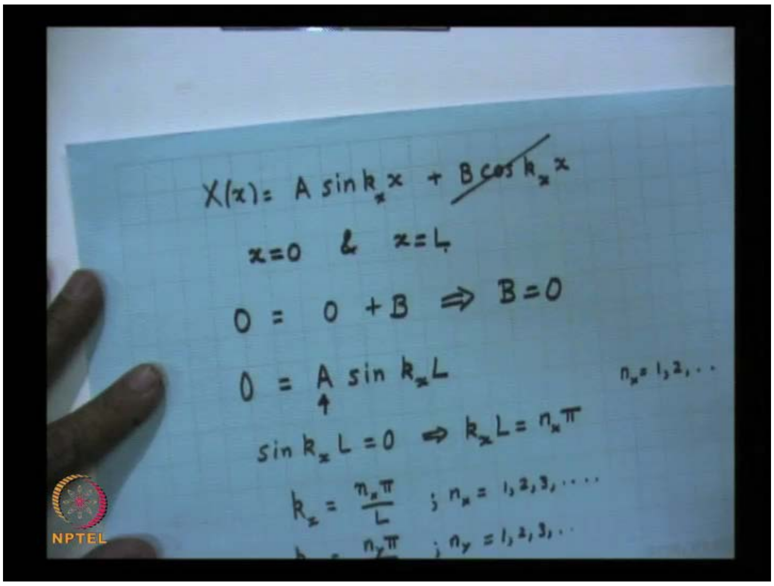

And the solutions are the solutions are x of x is equal to a sine k x x plus b cos k x x. Now if this is the x axis then the wave function has to vanish on all points on the plane x equal to zero and on all points on the plain x is equal to l. So, the wave function has to vanish. So, if I put x is equal to 0, the wave function has to be 0. So, 0 must be equal to this is 0 plus b at x equal to 0. So, therefore, this will give me b equal to 0. So, this term goes out b equal to 0.

Then, we have at x is equal to l would the function must be 0. So, 0 is equal to a sin k x l as we had done quite sometimes earlier there are now two possibilities one is that either a is 0 or sin k x l is 0. If a is zero, then the wave function is zero at all places. So, psi is equal to 0 everywhere. That is known as the trivial solution. So, a cannot be zero so, we can have only sine k x l must be 0 and. So, therefore, which will imply k x l is equal to n x pi, where n x will be not zero because again if it is zero then k x is zero if k x is zero then the wave function is zero everywhere. So, that is again a trivial solution. So, you have the allowed values of k x are n x pi by l where n x is equal to one two three four.

Similarly, we have solved this equation because the y equation is one over y d 2 y by d y square is equal to minus k y square. So, that will lead to the will lead to the equation d 2 y by d y square plus k y square y of y is equal to 0. Once again, we will have sine and cosine and exactly the same thing. So, we will find that they allow values of k y will be n y pi by l that n y also takes the same set of values one two three etcetera and finally, the z component the z k z will be n z pi by l and n z takes also this thing.

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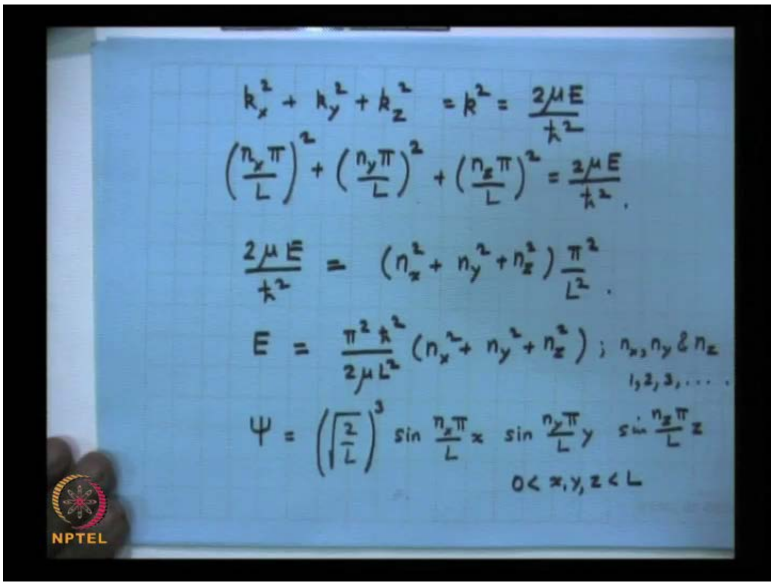

So, you will have if you recollect that therefore, we had k x square plus k y square plus k z square was equal to k square this is equal to 2 mu e by h Cross Square now we find that k x takes discreet values. So, we have n x pi by l whole square, plus n y pi by l whole square plus n z pi by l whole square. This is equal to two mu e by h cross square. So, I bring it to the left hand side. So, we have two mu e by h cross square is equal to is equal to is equal to n x square plus n y square plus n z square times pi square by l square. We get the remarkable result that the energy levels at discreet and you will have pi square h cross's square by two mu l square n x square plus n y square plus n z square, where n x n y and n z they can, each take the value one two three. So, these are the discreet values of the energy and corresponding to each set of n x n y n z. We have a wave function and that is that is k x was equal to if you remember k x is n x pi by l. So, the wave function will be some normalization constant which I can show to you equal to under root of two by l whole cubed sin of n x pi by l into x sin of n y pi by l into y sin of n z pi by l into z this is 0 less than x y z less than l inside the box.

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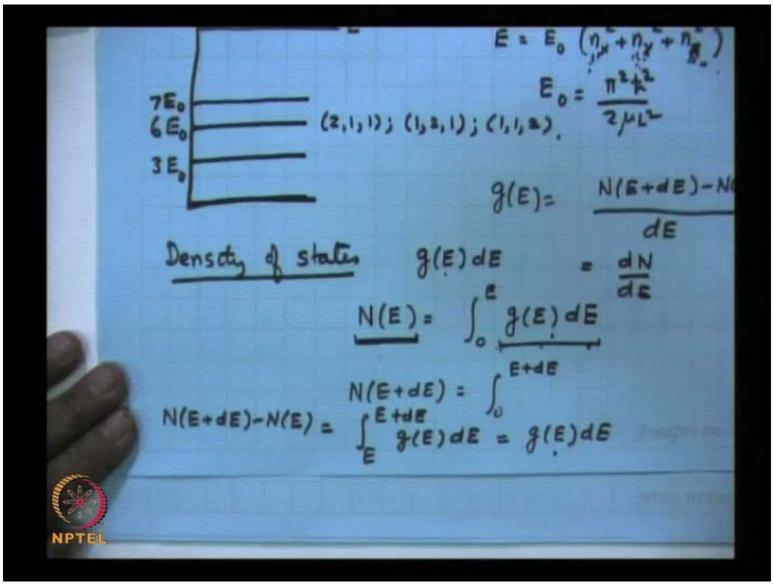

So, these are the normalized wave functions and these are the discreet states. So, what is the ground state value the ground state value is n x is equal to one n y is equal to 1 n z is equal to 1. So, three pi square h cross square by 2 mu l square. So, you have here if you if you plot this e then the ground state is something like say three E 0 where you see the allowed value of E is say E 0 n x square plus n y square plus n z square E 0 is equal to pi square h cross's square by 2 mu l square. So, if n x is 1 n x y is one n x z that is the ground state. So, this is 1 plus 1 plus 1 that is 3. Then you will have 2 11 1 2 1 11 2 that state will be three fold generate state and this will be four plus one plus one that is 6 E 0.

So, this will be 2 1 1 1 2 1 and 1 1 2 and then you can have 3 1 1 that is 7 E 0 3 1 1 1 3 1 and 1 1 3 so, that is 7 E 0 and so on. You can write down the various states very quickly there will be for a given value of e there will be many sets of integers whose sum of square is a given number. So, I have been able to obtain, the exact solution for a particle in the three dimensional box for a electron confined in a cube volume l cube and have been able to obtain the exact wave functions and the exact energy levels and there are infinite number of states.

What I would like to calculate and what is of extreme importance in solid state physics in astrophysics and in many areas is to calculate the density of states that is, density of state meaning when the energy level becomes very large states have very closely spaced and there are very large number of states.

And g of e d e represents the number of states, whose energy lies between E and E plus d E. Once again g of E d E represents the number of states whose energy lies between e and E plus d E. So, let us suppose I want to find out the total number of states. Which had energy less than E then N of E will be equal to 0 to E g of E d E.

This is the density of states and this is the total number of states. Whose energy is less than E that is a difference in dimension between N of E and g of E 1 has to be a little careful g of E represents the density of states. So, that g of E d E represents the number of states, whose energy lies between E and E plus d E and N of E will represent the total number of states whose energy is less than e. Now that the quantity and if I am able to find out N of E then of course, I can differentiate N of E for to obtain g of E because N of E is given by base. N of E plus d E I can write this down as 0 to E plus d E and if I subtract one from the other. So, n of E plus d E minus N of E is then equal to from E to E plus d E g of E d E. So, in this small interval this becomes equal to g of E d E.

And so therefore, g of E is equal to N of E plus d E so, g of E will become N of E plus d E minus N of E divided by d E so, d E is extremely small than d N by d E. So, if I am able to find out N of E then a simple differential will give me g of E. So, in next lecture, what I will do is that I will obtain an expression for N of E and obtain the density of states and thereby we will be able to obtain the property of the electron inside a metal. A similar kind of analysis can be applied, even for the electrons inside a whitewash star. So, we will probably discuss that very briefly thank you.