Introduction to Quantum Mechanics
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Lecture - 01
Solution of the Schroedinger equation for a particle in one and 2 delta function potentials

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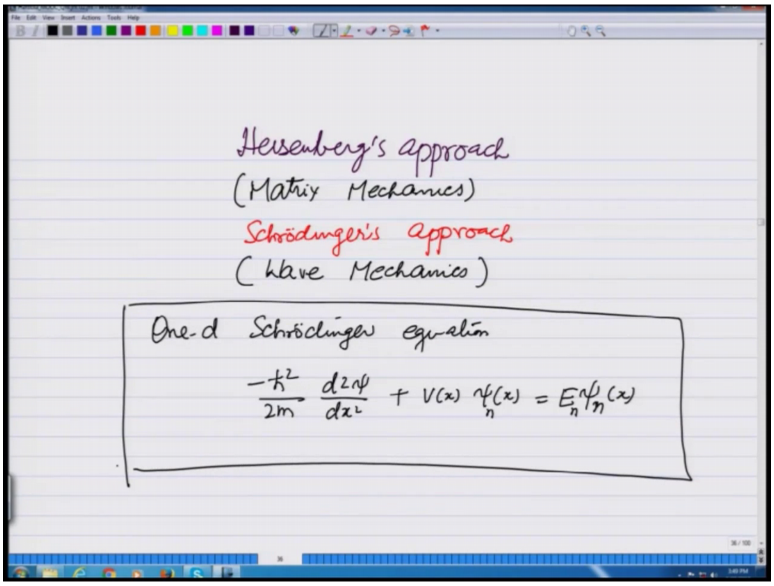

What we have done so far is the version which is known as the Heisenberg's approach which is essentially what we called matrix mechanics and as one of the students in the forum also pointed out it does become difficult after certain simple problems and the other version will not about is the Schrodinger's approach which is nothing but what I will call wave mechanics and its considers particles has having associated with sensor for the wave function the one d Schrodinger equation. And we have solved it in 2 cases is written as minus h cross square over 2 m d 2 psi over d x square plus V x psi x equals E psi x and I am going to put in n here I as subscript to show that these are I can functions which satisfied boundary condition.

So, the satisfaction of boundary condition gives you the Eigen values energy E n and the corresponding Eigen functions. So, this is the approaches that we are going to now follow in the coming lectures and apply Schrodinger equations solve problems some standard and some non standard wave, we are going to use numerical approach to solve the problem we are going to start with very simple problems and slowly increase the difficulty level.

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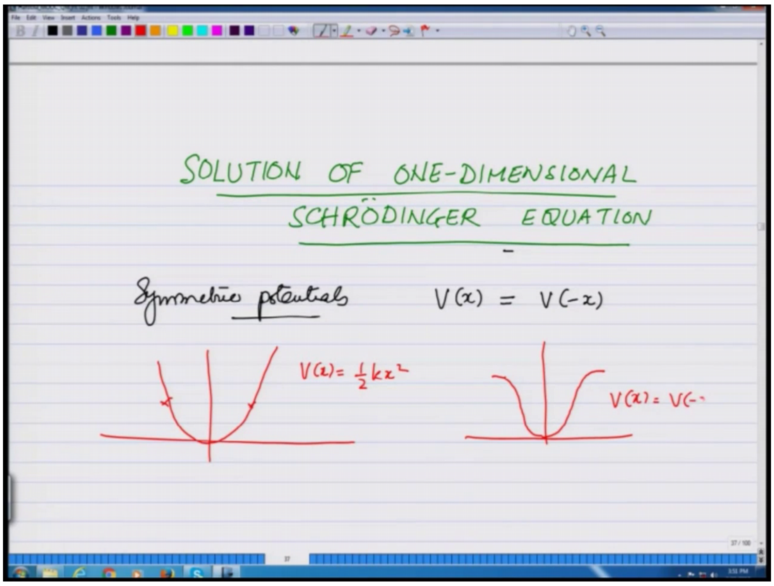

So, from now onward what we are concentrating on is the solution of the timing one dimensional Schrodinger equation and since I am starting the simple problems, I will start with something called the symmetric potentials and what I mean by that is that if I go from positive x to negative x; the potential does not change.

So, V x is V minus x for example, if I take a potential which is simple harmonic that is V x equals 1 half k x square its same for the negative axis and the positive axis. So, this is a symmetric potential any potential that has exactly the same value on 2 sides of the y axis is a symmetric potential and does not confine to potential being only positive.

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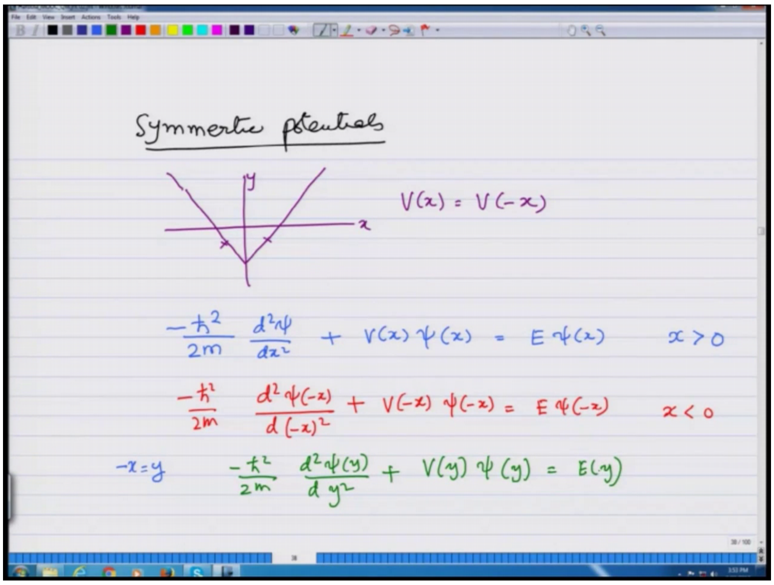

So, let me just write some more examples. So, I am talking about symmetric potentials, for example, I could write this potential which is again the same on 2 of sides the y axis, this is also V x equals V minus x, this is also symmetric potential and why I am focusing on these write now is that they have a special advantage they provide special advantage while solving the Schrodinger equation let me look at the Schrodinger equation for such potentials. So, the Schrodinger equation is this plus V x psi x equals e psi x, let me write this only for x greater than 0, the equation for x less than 0 is therefore, going to be from this equation minus h crosses square over 2 m d 2 psi minus x over d minus x square plus V minus x psi minus x equals e psi minus x, all I have done is change x 2 minus x.

Now keep in mind that minus x square is same as x substitute minus x equals y then the equations becomes minus h crosses square over 2 m d 2 psi y over d y square plus V y psi y equals E y. So, this is basically going back and forth important thing, now is going to be that when I take this equitation.

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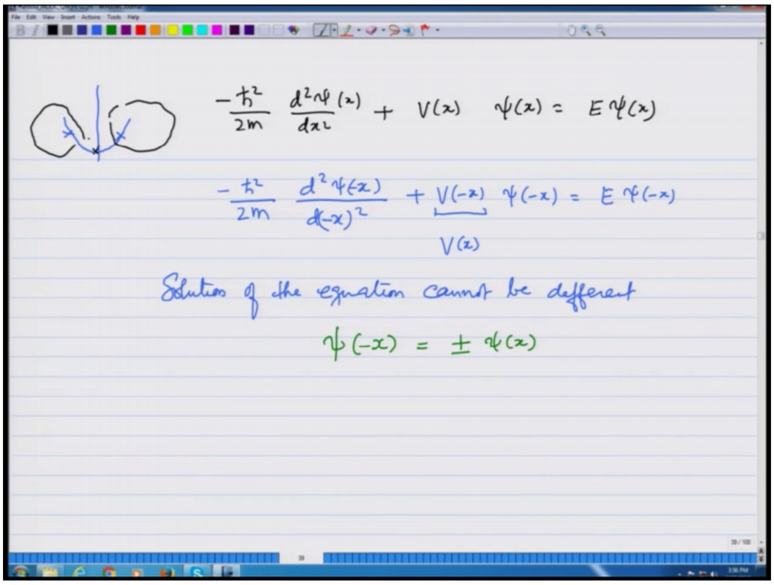

Minus h crosses square over 2 m d 2 psi d x square plus V x psi x equals e psi x and change to the other side of the y axis. So, that is some potential is there an instead of writing here I want to write the equation for the other side this is going to be minus h crosses square by over 2 m I can just change signs psi x minus sign here over d minus x square plus V minus x psi minus x equals e psi minus x this same as V x.

So, since V is the same on the both sides the solution of the equation cannot be different write V x and V minus x are one and the same, think there will be exactly the same number as the function of. So, as the function of minus x, we gives exactly same number as the function of x. So, solutions cannot be different at this differ by constant.

So, psi minus x is going to be plus or minus psi x, I choose that constant to be one even if I take to some constant c I can always take it that to be one multiplied by constant does not really change this solution, important thing is that if V minus x and V x other same then the way solution evolves as the function of x on the right hand sides. So, let me show this in black the way this solution would evolve from a boundary condition, here 0 to the right hand side would evolve exactly in the same way on the left hand side and therefore, the 2 solutions are going to be changed by only by a factor of plus or minus 1.

So, this is an important property of the wave function for symmetric potentials which I am going to make use of.

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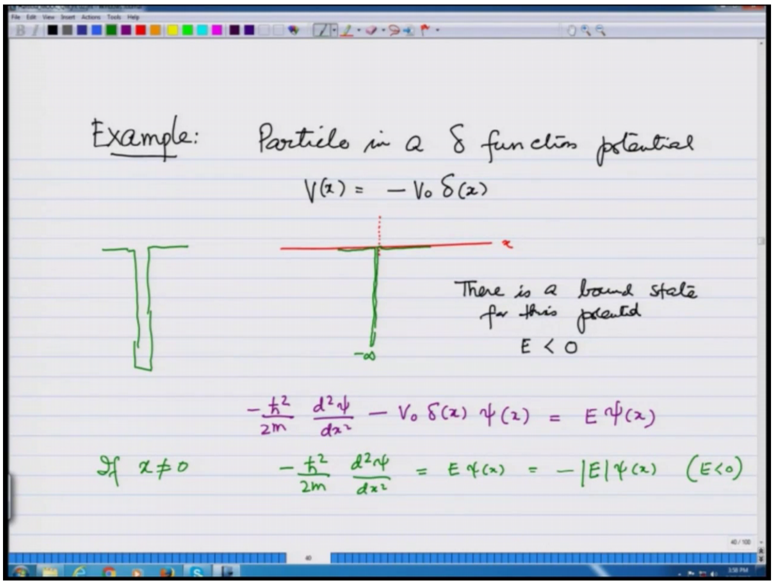

So, in solving Schrodinger equation let me take the first example of particle in a delta function potential and what I mean by that is that the potential V x is equal to minus V 0 delta of x, how does this potential look? This potential is going to look like this, if this is the x axis, this is the y axis, it is going to be very deep at x equal to 0, infect going to minus infinity and 0 everywhere else this could be a representation of a potential which is very deep an and has very small width classically whether this can a ford a bound state or not we do not know, but quantum mechanically I am going to show you that this afford someone state.

So, there is a bound state for this potential; what do we mean by that bound state; that means, total energy e is going to be less than 0 the particle is going to be bound near e delta function.

Let us see how it is that come of bound. So, the Schrodinger equation for this is minus h cross square over 2 m d 2 psi over d x square minus V 0 delta x psi x equals e psi x and what; that means, is that if x is not equal to 0, then I have minus h cross square over 2 m d 2 psi over d x square is equal to e psi x and this means minus modulus of e psi x because e is less than 0 and what will happen at x equal to 0, I show you in a minute.

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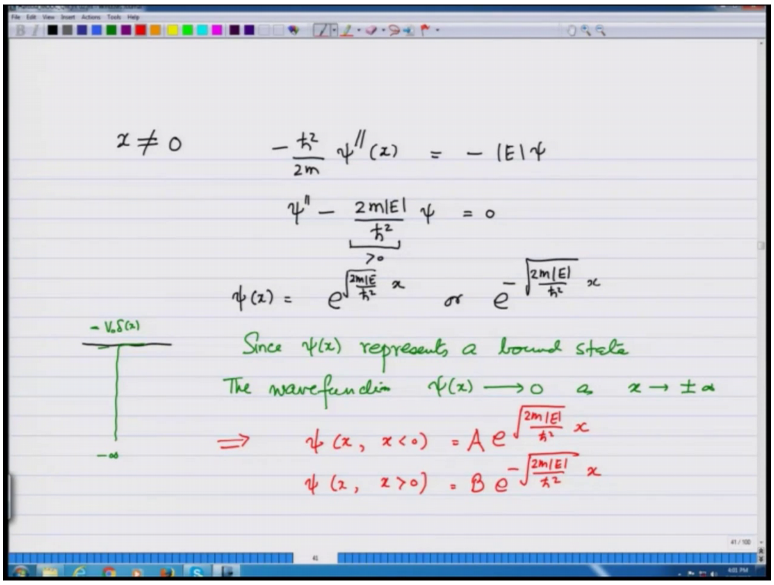

So, for x not equal to 0, I have minus h cross square over 2 m psi, let me write it is double prime for the second derivative x equals minus modulus of e psi and therefore, psi double prime minus 2 m E over h cross square this is modulus psi equals 0. This is a positive quantity and therefore, you can immediately write the solutions. So, psi x is going to be e raise to square root of 2 m mod E over h cross square x or e raise to minus square root of 2 m mod E over h cross square x that is the solution since this is the bound state right let me make the potential again.

So, that it is you know mine; what we are solving for the potential is right here, very deep minus infinity this is V naught delta x and 0 everywhere else since psi x represents bound state; that means, the wave function psi x must go to 0 as x goes to plus or minus infinity; that means, there is a almost 0 probability of finite the particle far away from the potential.

And this immediately implies that psi x for x less than is 0 is going to be e raise to square root of 2 m mod E over h crosses square x with some constant A, in front and psi x, x greater than 0 is going to be some constant B e raise to minus square root of 2 m mod E over h cross square x, I have deliberately chosen these constants to be different because I do not want to make a point.

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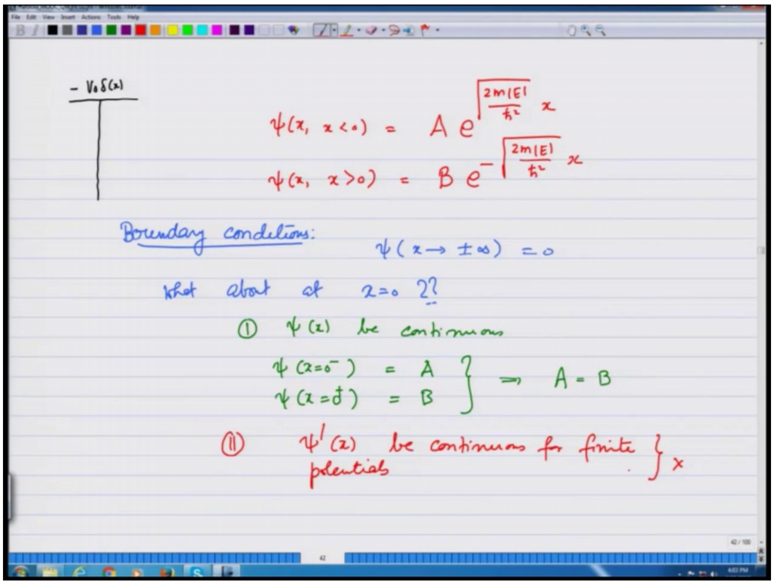

So, in this case that we are considering a delta potential V naught delta x potential, these solutions are psi x x less than 0 equals some constant A e raise to square root of 2 m mod E over h cross square x and psi x x greater than 0 is equal to some constant B e raise to minus square root of 2 m mod E over h cross square x what about boundary conditions psi x tending to plus or minus infinity is equal to 0 is automatically satisfied.

Now, we have written the solution for x greater than 0 and x equal 0 what about at x equal to 0 is the equation, recall what we asked what we demanded from the solution of the Schrodinger equation 1 psi x be continuous and this means at x equals 0, the value should be the same from both sides.

Now, if you look at the solutions psi x equal to 0, if you come from the left hand side that is x less than 0, this is A and psi x equals 0 is B, if you are come from the right hand side. So, I will denote that; I will write the upper 1 as 0 minus 0 plus and the 2 should be the same and this implies A equals B number 2, we had demanded that psi prime x that is the derivative of psi with respect to x be continuous for finite potentials.

Now, in this case a particular case that we are dealing with the potential is not finite at x equal to 0 it goes to minus infinity therefore, this condition has to be replaced by some other condition and we will do that now.

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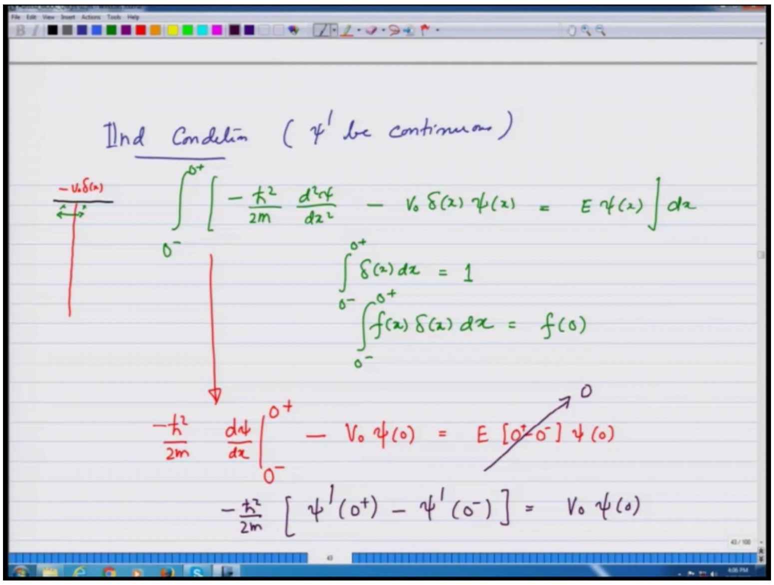

So, the second condition which is psi prime be continuous, it is going to replace by something else and let us see how that is replaced we have the Schrodinger equation d 2 psi 2 psi over d x square minus V 0 delta x psi x equals e psi x.

Since the discontinuity is at x equals 0, let me integrate this equation with respect to x from 0 minus to 0 plus what does that mean? Pictorially if this is the potential minus V 0 delta x I am integrating from slightly left from a to slightly right I am integrating in this interval shown by green here; that means, its include the delta function and keep in mind that integration of delta x d x from 0 minus to 0 plus is 1 any function f x delta x integrated over from 0 minus to 0 plus is equal to f at 0.

So, therefore, what do I get from the equation minus h cross square over 2 m when d 2 psi over d d x square is integrated I get d psi d psi by d x and this is from 0 minus to 0 plus minus V 0 psi 0 is equal to e sum is small interval which I can write as 0 plus minus 0 minus psi at 0 as the interval is made smaller and smaller. The right hand side is going to go to 0. So, the only conclusion I can draw now is that minus h cross square over 2 m psi prime at 0 plus minus psi prime at 0 minus is equal to V naught psi at 0. So, this is what the delta function does if the delta function was not there psi prime would have been continues, but because the delta function there is a discontinuity n psi prime and that is what leads to know the energy.

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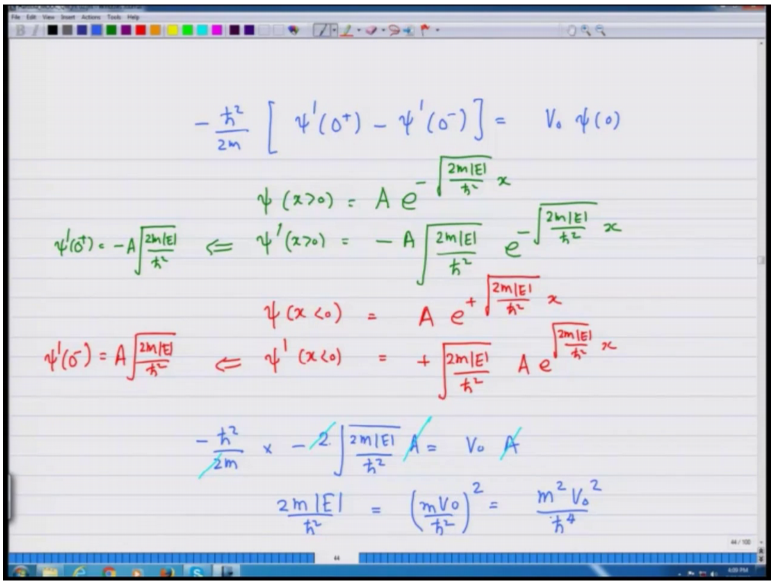

So, let us write this now. So, the boundary condition at 0 is now minus h cross square over 2 m psi prime at 0 plus minus psi prime at 0 minus is equal to V 0 psi 0. Now psi at x greater than 0 is nothing but e raise to minus square root of 2 m mod e over h cross square x and therefore, there is a factor a also psi prime for x greater than 0 is equal to minus a times square root of 2 m mod a over h cross square e raise to minus square root of 2 m mod a over h cross square x and psi x less than 0 is a e raise to plus square root of 2 m mod a over h cross square x and psi prime for x less than 0 is going to be equal to plus square root of 2 m mod e over h cross square a e raise to square root of 2 m mod a over h cross square x.

So, this immediately implies that psi prime 0 plus is equal to minus a square root of 2 m mod a over h cross square lower side immediately implies that psi prime 0 minus is equal to a square root of 2 m mod a over h cross square and psi 0 of course, A. So, if I substitute this in the equation above blue equation I get minus h cross square over 2 m times minus 2 square root of 2 m mod a over h cross square is equal to V 0 times A, this A also floating round here and we cancel this a and I get 2 m mod e over h cross square is equal to m V 0 over h cross square is 2 also cancels. So, this is equal to m square V 0 square over h cross raised to 4.

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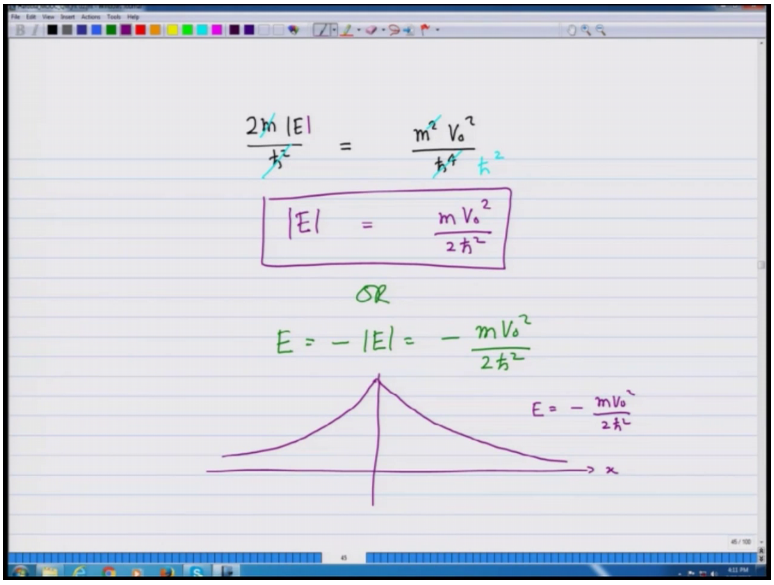

So, what I have is from the boundary condition 2 m mod A over h cross square is equal to m square V 0 square over h cross raise to 4, we can again cancels in terms this gives me h cross square 1 m cancels and therefore, I get mod of E equals m V 0 square over 2 h cross square or energy E which is equal to minus mod E is equal to minus m V 0 square 2 h cross square; how does the wave function look the wave function if I plot it and on the x axis is exponentially decaying on the right hand side exponentially decaying on the left hand side d psi by d x is discontinuous at x equal 0 and the energy e equals minus m V 0 square 2 h square that is the solution for a particle moving in a delta function potential you can see it is bound and it has energy just slightly negative that is why it is bound and the wave function is exponentially decaying on the 2 sides.

There are no other bound states in this potential. So, this is the answer for this if you want to normalize the wave function right. So, you have to see now is calculated the wave function psi x.

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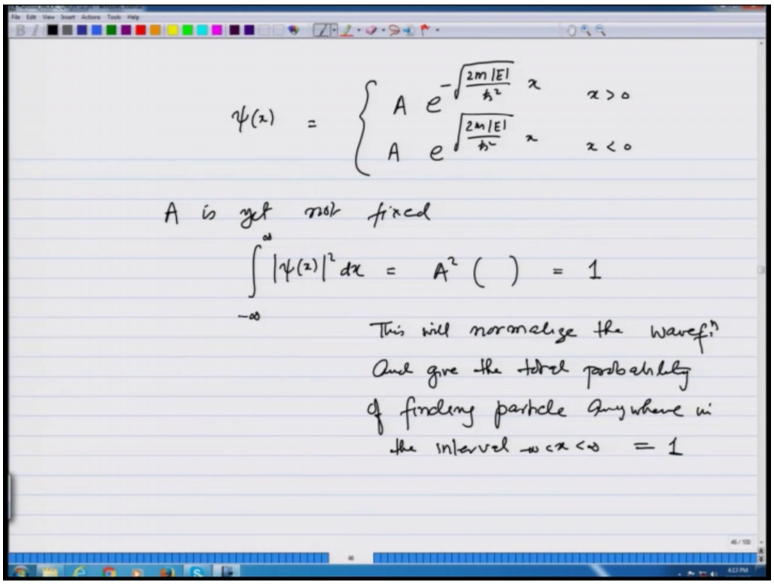

Let me write it in 1 bracket e; e raise to minus square root 2 m mod E, we have calculated over h cross square x mod x greater than 0 A e raise to square root of 2 m mod E over h cross square x or x less than 0 A is yet not fixed if you want to fix it, what we will do is we will take psi x square integrated from minus infinity to infinity which will give me sum A square times sum constant and fix it equal to 1 and this will normalize the wave function and give the total probability of finding particle anywhere in the interval x minus infinity to infinity to be equal to 1; then I have a normalized wave function.

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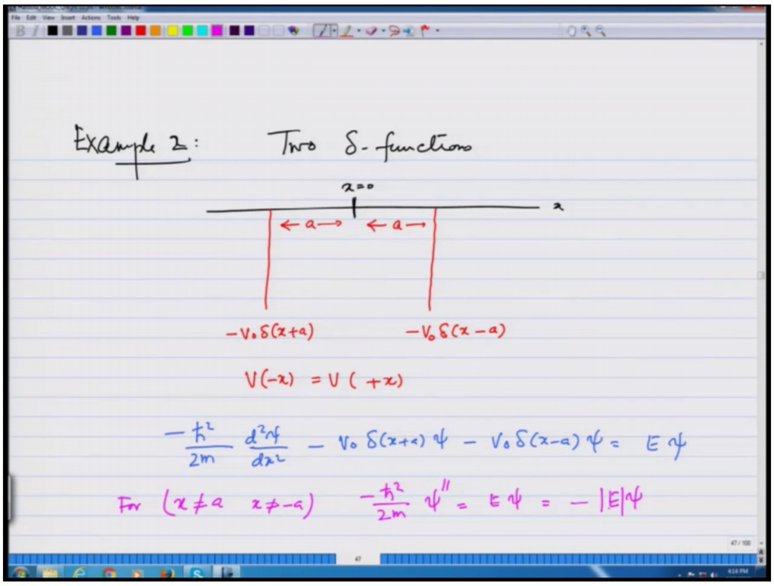

So, this is a very simple problem to start with the wave out generalized this would be 2. So, let me take example 2. So, the way to generalize this week 2 delta functions. So, in this case, I have the x axis, this is x equal 0 and 2 make the problem simple, what I will do is, I will put the delta function symmetrically about x equals 0 and both are the same V naught delta x minus a and this will minus V 0 delta x plus A. So, again the potential is symmetric V minus x equals V plus x and therefore, the solution is going to be either symmetric or anti symmetric in this case it. So, happens that we get 2 bound states and let me show you how. So, the Schrodinger equation is h cross over 2 m d 2 psi over d x square minus V 0 delta x plus a psi minus V 0 delta x minus a psi equals e psi.

For x not equal to A or x not equal to minus A together equation is minus h cross square over 2 m psi equals e psi double prime psi which is minus modulus of e psi.

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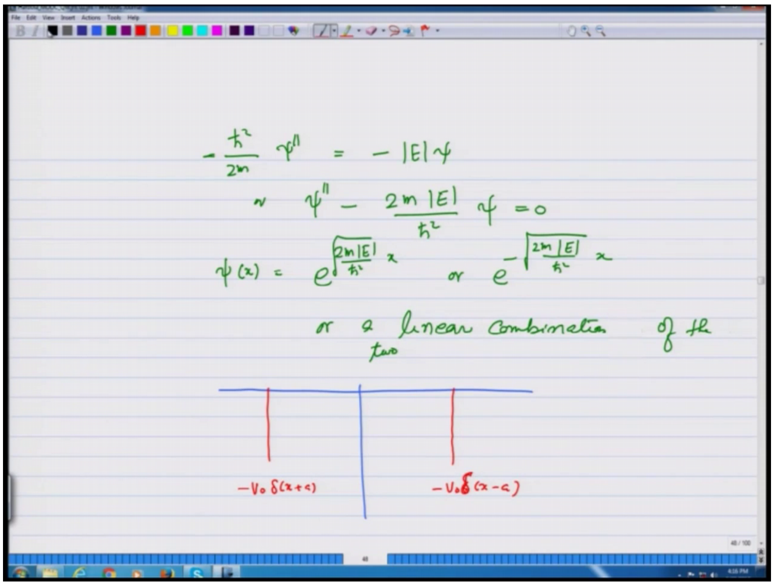

So, the equation I am solving again is h cross square over 2 m psi double prime is equal to minus mod a psi or psi double prime minus 2 m mod a over h cross square psi of 0. So, solutions again are e raise to 2 m mod e over h cross square square root x or e raise to minus square root of 2 m mod E over h cross square x or a linear combination of the 2 now let me show you how you form this linear combination.

Even if you do an elaborate exercise you will get exactly the same answer. So, this is my x axis the potential is symmetric minus V naught delta x plus a minus V naught delta x minus a.

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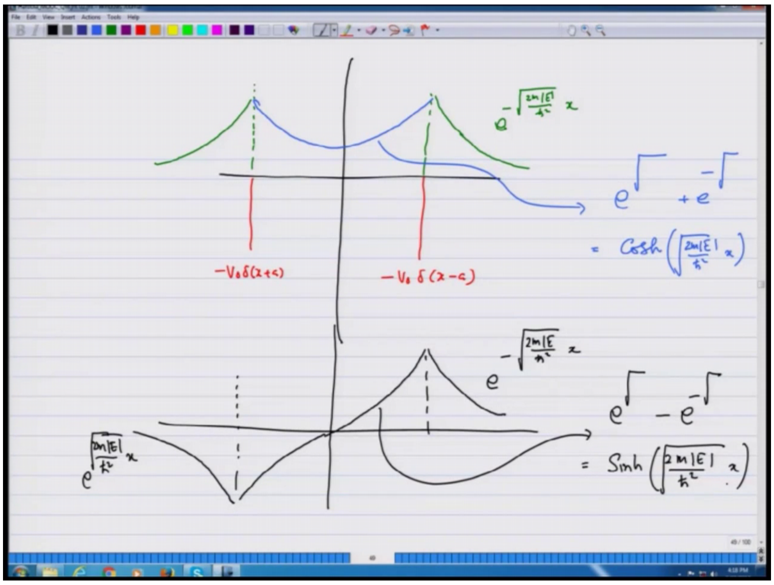

Now, look not the wave function the upper side these are the potentials minus V naught delta x plus a minus V naught delta x minus a and on the right side the potential as to d k exponentially e raise to minus square root of 2 m mod E over h cross square x. So, on the x positive side, the solution has negative power of the x exponential on the left hand side. The solution again as to d k because the bound state in between I am going to have either symmetric or anti symmetric solutions the symmetric solution would be linear combination with two. And let me show on the lower side anti symmetric solution and that would be the solution decaying on one side and anti symmetric solution has to go to 0 necessarily through 0. It has to be 0 at the 0 and again explanation on the other side, this is e raise to minus square root of 2 m mod E over h cross square x. This is e raise to square root of 2 m mod E over h cross square x and in between it is an anti symmetric combination.

Symmetric combination is going to be a raise to the square root whole thing plus e raise to minus square root over thing which is nothing but the hyperbolic cosine function x and the lower case this is going to be an anti symmetric combination. So, is going to be e raised to square root of this whole thing minus e raise to minus square root of this whole thing and this is going to be sin hyperbolic of 2 m mod E over h cross square square root of h. So, I give you a qualitative argument based on symmetry how the wave function should look like as to what it linear combinations of these 2 solutions would be for the symmetric and anti symmetric wave function.

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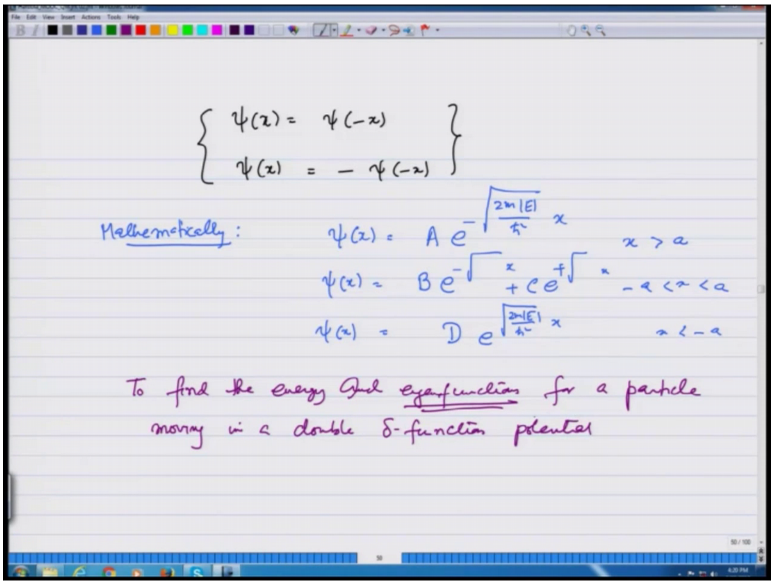

So, in the first case psi x equals psi minus x and the second case psi x equals minus psi minus x. This is a qualitative argument based on the symmetry if you on do it mathematically, what you would say is psi x is equal to A e raise to minus square root of 2 m mod E over h cross square x for x greater than a psi x is equal to sum constant B e raised to minus square of whatever this quantity is plus C e raise to plus square root of this whole thing x x for x between a and minus a and psi x equals from D e raise to square root of 2 m mod E over h cross square x for x less than minus a and then match the boundary condition that the psi we continuous at the boundary and so on and then you will find the solution.

Now this I will be assigning you as an assignment problem to find the energy and eigenfunctions actually eigenfunctions I have already written for a particle moving in a double delta function potentially.

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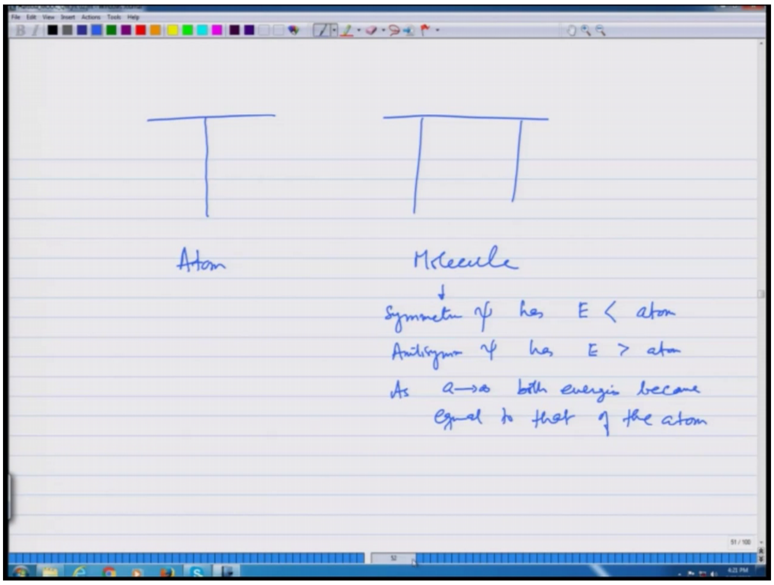

Significance of this problem is that a single delta function is like an atom and a double delta function is like a molecule and in this case, you would find that symmetric psi has energy lower than the atom. So, that that is why molecules that formed and anti symmetric psi has energy greater than the atom and as a tends to infinity both energies become equal to that of the atom.

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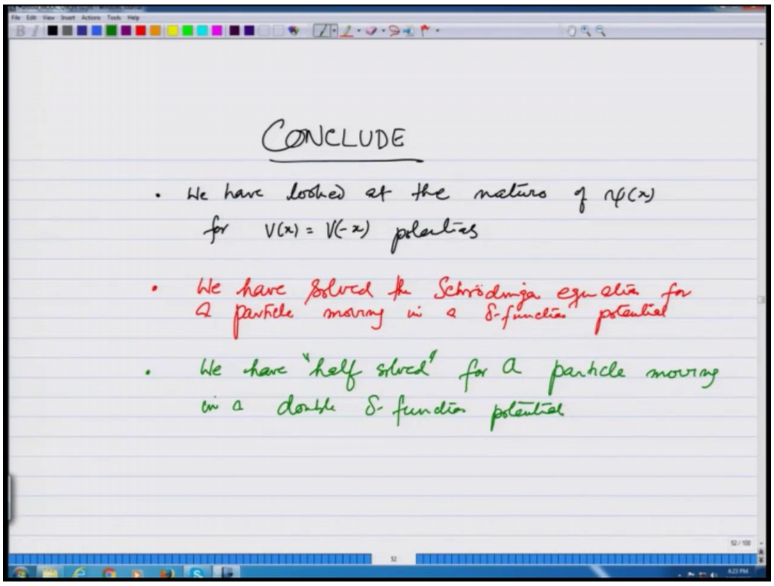

So, let me conclude this lecture by stating that we have note at the nature of psi x for V x equals V minus x potentials 2, we have solved the Schrodinger equation for a particle moving in a delta function potential and third we have half solved. And I will give you western as the assignment for a particle moving in a double delta function potentially.