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Lecture - 02
Quantum Mechanics: Particle in a Box

All right. So, continuing on from you know where we left off in the previous lecture. We will look at the Schrodinger's equation in Quantum Mechanics. We basically introduced it in the previous lecture, but from this point on we will see how to actually use the Schrodinger's equation and what can tell us about the behaviour of the wave particle in certain systems.

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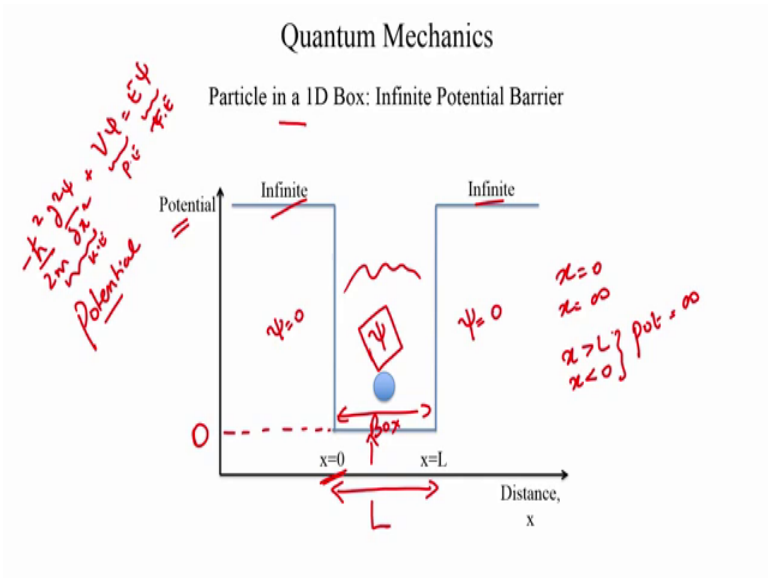

So, the first example or the application for our Schrodinger's equation would be through an example, which is quite popular and which is something called as a particle in a one dimensional box, ok. And what we have here is the profile of the potential versus the distance.

Now, although we keep mentioning the word potential, and I do keep using the term potential, I would like to emphasize that this term in Schrodinger's equation which is minus h square by 2 m dou square psi by dou x square plus V psi is equal to E psi. This term correspond to the potential energies we are equating energies, ok. So, we are saying that this is the kinetic energy, this is the potential energy and that is the total energy, ok.

But since the potential is has an is the equivalent of the potential energy, I would sometimes use the term potential I while talking about these concepts.

So, in this case we now have a potential profile that looks like as shown, and the particle or the wave function exists somewhere in this region from x equal to 0 to x equal to infinite. But the potential profile is such that between this region of x equal to 0 to x equal to L the potential has a value of 0.

And in the regions outside x equal to L and below x equal to 0 the potential has a value of infinite, which implies that the electron or the particle that we are considering has to have an infinite amount of potential energy in order to be located in these regions, ok. It has to have an infinite amount of energy to be located in the regions outside this little valley and this valley is what we call as the box. And as per this definition this valley has got a length or the size of the box is of length L that the coordinate system being placed x equal to 0 at this boundary and x equal to L being located at this boundary of the box.

Now, since all these potentials are infinitely large we say that the wave function it is impossible for the particle to be present located in to be located in those regions and for this example the particle remains very much confined to the box, ok. So, the magnitude of the wave function, so since we are talking about the wave particle the magnitude of the wave functions in these regions is 0 whereas, the magnitude of the wave function or the made through the wave function inside the box is what is to be determined.

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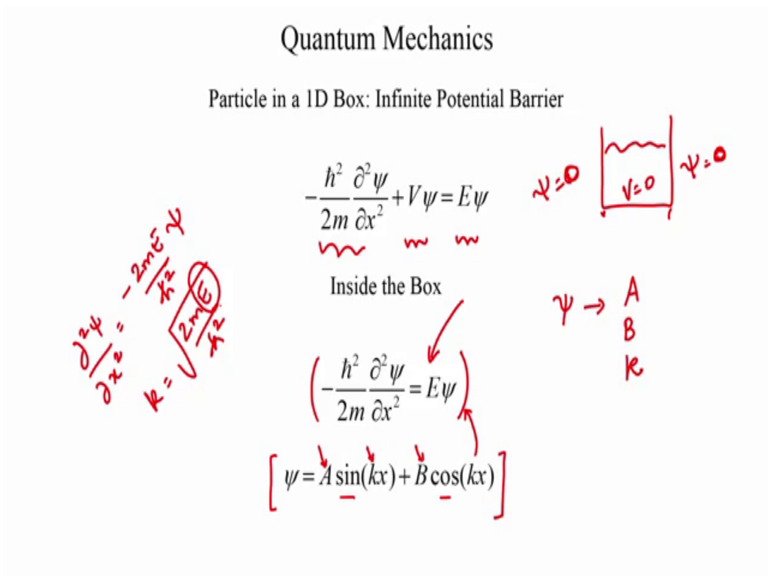

So, we can now, write Schrodinger's equation for this example of a particle in a box and say that this is the kinetic energy that is the potential energy, and that is the total energy and for the region that is inside the box the potential energy is 0, ok. And therefore, Schrodinger's equation reduces to this simple form and outside the box as we mentioned it is not possible for the particle to exist since it would require an infinite amount of energy and we say that the wave function has got a amplitude of 0.

Now, the general solution to an equation or second a differential equation of this kind is given by defining the wave function as a summation of sines and cosines. So, we say that the wave function is A sin k into x plus B cosine k into x, where A is nothing but a constant coefficient and B is a constant coefficient and k is another coefficient that needs to be determined, ok. So, from this point on they are going to apply the correct boundary conditions to try and define the wave function of the wave particle inside the box more accurately and in particular we need to identify the parameters A, B and k. Now, k can also be seen can be seen to be related to the energy right from Schrodinger's equation.

So, if we were to rewrite the differential equation as dou square y by dou x square is equal to minus 2 m E by h bar square into psi, the value of k is related to the energy and it is 2 m E by h bar square. But we would now, like to identify a further relation, of k particularly with regards to the geometry of the box and then use that relation to identify the nature of the energy.

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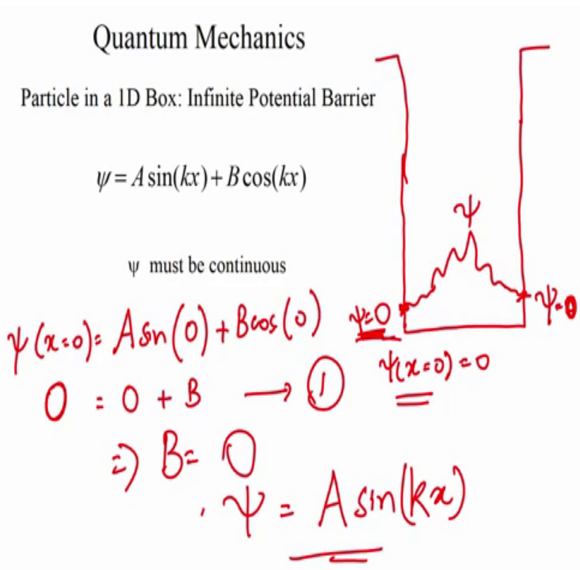

Now, since this is a general solution let us apply the property that the wave function must be continuous, ok. So, this was the second property of the wave function that we discussed, ok. So, which implies that if I were to consider these two boundaries, which is there is some wave function here, we do not know what the way we what the function is but it must be continuous which means that if I were to go to this boundary, ok.

The value of the wave function just inside this edge must equal the value of the wave function outside this edge, ok. And similarly if you go to the other side the value of the wave function inside this edge must value must equal the value of the wave function outside. And since we said that the wave function does not exist in this region, the wave function is essentially 0, the probability of finding a particle outside this box is 0. So, that is the statement we made and the argument also the box is infinitely high, ok. So, it is an in surmount insurmountable cliff. So, you have the wave function being 0 on the outsides and therefore, the wave function at x equal to 0 must be equal to 0 that is the continuity, that is the continued continuous made through the wave function.

So, we first apply this condition that psi at x equal to 0 is 0. So, psi at x equal to 0 is A sin of k into x, which is 0 plus B cosine of k into x which is 0, ok. And this turns out to be 0 plus B is equal to the wave function at x equal to 0. And since this value the wave function takes a value 0 we need this to be the first condition which implies that my B is 0 therefore, my wave function is or the form A sin of k x. So, for any x since B is 0 the cosine term does not exist. So, this is the wave function. So, you have identify we have reduced the wave function from this very generic sine and cosine terms to just having A sinusoid term.

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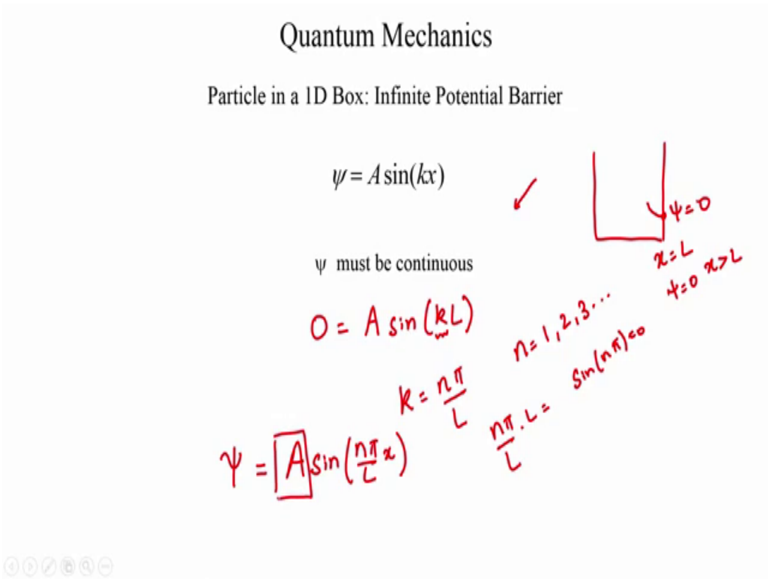

So, now let us apply the boundary condition on the other side of the box, which is at x equal to L. And at x equal to L again we find that the wave function must be equal to 0 since the particle cannot exist on or the wave particle cannot exist on the in the regions where x is greater than L.

Now, applying that boundary condition at x equal to L we say that this is the value or the magnitude of the wave function is 0 in at sin k L. Now, what are the possible solutions? They could have A to be equal to 0, but that would simply that would be a trivial solution as it simply say that the wave function does not exist. So, we will ignore that solution because we also have the possibility of a solution, where k can be an integer times pi by L, where n could be positive integers 1, 2, 3 and so on.

And n pi by L into L is a integer times pi and sine of an integer times pi is 0. Therefore, this way function has now become more specific we can define the wave function more clearly by applying the boundary condition at x equal to L and saying that the wave function is A sin of n pi by L into x. Now, all that remains is to identify A using that value of k.

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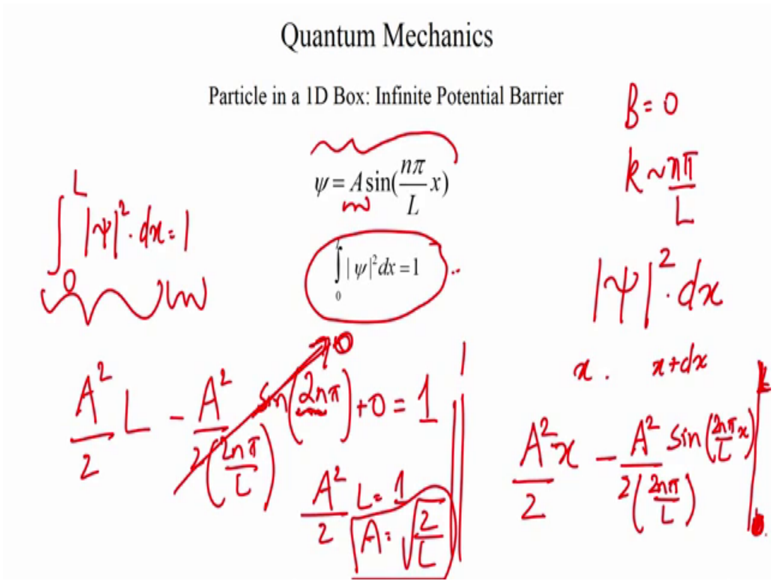

So, we have now identified B to be equal to 0 we have identified k to have the form of n pi by L, where n is an integer. So, the wave function has now reduced from this very general expression of containing sines and cosines its, now reduced to this it has to be other form of A sine n pi by L into x. Now, the only thing is left to be determined is A and we do that by using the condition that the particle must exist somewhere, right.

So, if you remember psi square was the probability density function for the particle, and psi square dx is the probability that the particle exists between x and x plus dx.

So, therefore, the probability that the particle exists somewhere inside the box, we have already said that it does not exist outside the box which implies that the particle must be existing inside the box. So, the probability that the particle exists somewhere inside the box, is basically the summation that the summation of all these little minuscule probabilities, which is simply the integral simply stating that the integral from 0 to L of all these little probabilities is 1, ok. So, this is the probability that the particle exists somewhere inside the box and that is guaranteed to be 1, according to this experiment.

So, this is the next condition that your general psi must satisfy. So, what does this become? So, it implies that from 0 to L, if I take A square sine square n pi by L of x then this must be equal to 1. Now, we write you can write your sine square, ok. So, let us say you have a general sine square alpha you must note that cosine of 2 alpha is cos square alpha minus sine square alpha or in other words its 1 minus 2 sine square alpha. Therefore, my sine square of any angle alpha is one minus cosine of 2 alpha by 2, ok.

So, we represent the sine square using this particular relation and what that gives you is that this integral is nothing but A square 1 minus cosine of 2 n pi by L x the whole thing divided by 2. And we need this to be equal to 1; we need this to be equal to 1, ok.

Now, this integral is simply A square by 2 into x, ok. So, this is all with respect to dx sorry I have missed that out, so here integrating with respect to x everywhere. So, this is the first term is going to be A square into one by 2 dx which is A square x by 2 minus you have A square by 2 into your 2 n pi by L into sine of 2 n pi by L into x, ok. And the boundary conditions are from 0 to L. So, the first term if I apply these boundary conditions it is this integral limits sorry these (Refer Time: 14:47) not the boundary condition sorry I mean the in the limits of integration are from 0 to L.

So, if I apply these limits, what do you get? The first term, the first term becomes A square by 2 into L and 0 just results in 0. And the second term when I throw in an L there you should get minus A square by 2 into 2 n pi by L sin of 2 n pi I mean I throw in a 0 there I just get 0, so minus 0, ok. So, this entire term must be equal to 1. Now, you see that since this is an even integer times pi this in is quite term will always be a 0, ok. So, therefore, this term also vanishes. And you are only left with the fact that A square by 2 into L is 1 or a is equal to square root of 2 by L. So, this is the outcome of applying this relation that the probability of the finding the particle somewhere inside the box is 1, ok.

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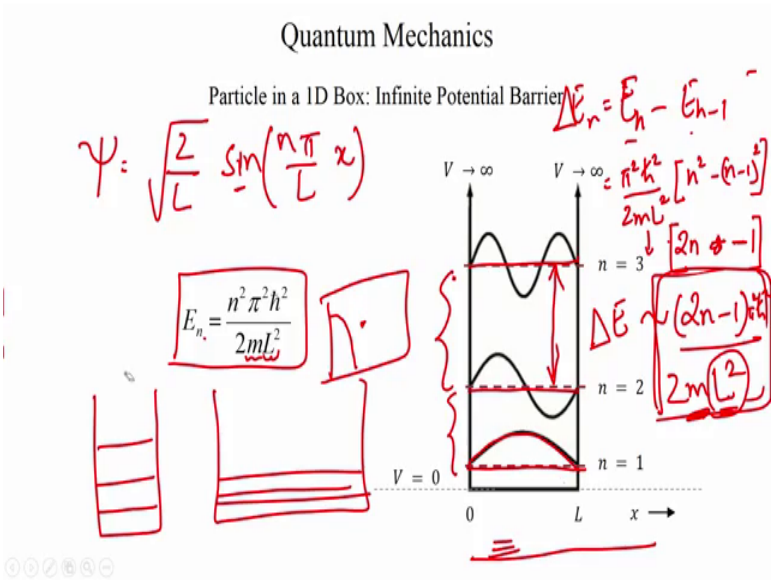

So, we can therefore, describe the wave function, ok. So, now, you have identified A to be square root of 2 by L you identified B to be 0 and you have identified k to be n pi by L, where n is an integer. So, k could take multiple values and they are all integer multiples of pi by L. So, therefore, my psi has now become square root of 2 by L sine of n pi by L into x. So, this is my wave function. So, now, we have identified we set out on this exercise try and identify A, B and k we have identified all 3 terms and we now have our wave function.

So, what this says is that. Firstly, note that the wave function is got A sinusoid term and it must it must always end on the boundaries it must always have a value of 0, ok. So, you will end up with the wave function looking like this, where at x equal to L by 2 if you take if you take the case of n equal to 1 firstly, you will have sine of pi by L into x and at x equal to L by 2 the this value takes a value 1 which is the highest value. So, you will find the, at n equal to 1 the wave function looks like this.

At n equal to 2 I have sine of 2 pi by L into x, and at x equal to 0 at x equal to L the value is definitely 0, but it is also 0 at a at x equal to L by 2. So, if I if my n is equal to 2 so this was the n equal to 1 case, if n is equal to 2 at x equal to L by 2 my wave function again takes a value 0 the amplitude takes a value 0 because sine of 2 pi by L into L by 2 is simply sine of pi which is again 0 but at x equal to L by 4 the amplitude is the highest, ok. So, you find that the wave function at n equal to 2 takes a takes a shape of this kind and you can continue drawing this you know for n equal 2, 3, 4, 5 etcetera. So, this is my wave function all right. So, that is the first point to know that the wave function is sinusoidal inside this box.

Now, let us now, try to calculate the energy of this wave function, and that is going to tell you a lot of interesting things. How do we calculate energy? So, since my minus x my Schrodinger's equation is minus x square by 2 m dou square psi by dou x square is equal to E psi, all right. And now, I know my psi accurately, so I am going to use this expression in the left term here.

So, the left hand side will now, become minus h square by 2 m, the first derivative of this will yield square root of 2 by L into n pi by L of x into n pi by L into cosine of n pi by L x, ok. So, if you look at what is d psi by dx it is square root of 2 by L, n pi by L cosine of n pi by L x and my d square psi by dx square is going to be minus square root of 2 by L into n pi by L whole square sine of n pi by L, ok.

So, we are going to use that term back here which is there is going to be a minus sign because the derivative of cosine is minus sign and that minus is going to cancel with this. So, I will put a plus sign it before this term into square root of 2, 2 by L into n pi by L squared sine of n pi by L into x. So, that is the left hand side and you will notice that this term here which is square root 2 by L into this sine is nothing but your wave function psi, ok. So, you might as well just write these two term, get rid of these two terms and just use, just use psi here and this is equal to E psi, ok.

Now, which means that my total energy is given by this expression here, which is n square pi square by L square h bar square by 2 m is my energy. For the when n takes a value where n takes only integer values, ok. So, this is the energy for some particular n. Now, the first thing which we notice here is that the energy cannot take any arbitrary value since n can only be integers, ok. So, if my n is 1 my energy is pi square h square by 2 m L square. If n is 2 my energy is 4 pi square h bar square by 2 m L square and so on.

So, the first thing to note is that the energy is quantized, you cannot have you cannot have this particle having an energy of let us say something in between. So, it cannot have nearly 1.5 pi square h bar square by 2 m L square because that violates the condition that n has to be an integer, ok. So, that cannot happen, all right. So, the first thing to note is that the energies are all quantized, ok. The second thing to note is that the energy is very strongly dependent on the size of the box it varies as 1 by L square. So, if you were to take a relation you know y is equal to 1 by L square and see how does y vary with L you will see its quite dramatic as L approaches 0 y climbs up very very large and as L starts increasing it completes completely comes down you know it reduces very very quickly, ok.

So, this depends on 1 by L square is quite dramatic. So, which means that if I have a box that is very narrow then the energy, energy the particle is very very large and the moment I start increasing the width of my box the energy the particle drops down, ok. So, let us let us note down these facts very neatly do forgive my reuse of the slide again and again, ok.

So, the first point we noted was that energy is quantized, ok. The second is that a small box implies large energy for the particle and a large box implies small energy for the particle. So, the energy scales is 1 by L square. Now, let us also look at the mass if the mass of the particle increases then my energy decreases, ok. So, these are all the absolute values of the energy, ok. But if I have to draw all the different energy levels, like as it is shown here. So, this is that n equal to 1 this was my wave function and n equal to 2 that is my energy, at n equal to 3 there is another there is another energy level and so on so forth, ok.

Now, if I were to draw all the energies and measure the distance or the energy gap between 2 subsequent levels, which is essentially which is essentially E n minus E n minus 1, ok. Now, I am looking at the delta E n, which is the energy difference between 2 subsequent energy levels. Now, according to this it should be pi square h bar square by 2 m L square into n square minus n minus 1 squared, ok. And if you were to just look at this expression it is nothing but 2 n plus 1 I am sorry 2 n minus 1, ok. So, the gaps between these which is my delta E, scales as 2 n minus 1 into pi square h bar square by 2 m L square.

So, the first thing to notice is as n increases the gaps between these two subsequent energy levels also increase. So, here you have a smaller gap and there you have a larger gap and n keeps increasing this gap will keep increasing. Now, the second thing to note is that as L or m increase the gaps will reduce, ok. So, for a large box not only is their total energy small the energy gaps between two subsequent energy levels is also small, for a large box.

And similarly the energy gap between two successful successive energy levels for a large particle the large mass is also small. And that is why when you have large bodies with large masses, ok, so even though they are composed of many particles if you avoid that if you just set that aside you know let us say it is all coherent and let us say it is just like behaves like one discrete large particle.

The spacing between the energies are so small that this massive entity can take almost any energy it likes, and therefore, you never get the feeling of something being quantized in your day to day experiences. So, if you were to take a billiard ball or a tennis ball and throw it you find that depending on the amount of energy you thrown classical mechanics tells you that it can always take any energy you like depending on how much energy throw into it, and that is not true in fact.

So, what this experiment is telling you is that if it is a discrete particle if you imagine even this large mass to be one particle. As the mass increases it would appear it would give you the illusion that the energies could be almost smooth and continuous, but in reality it is not and the difference, it is always discrete and that difference between 2 energy levels is given by this particular term here which we looked at this particular term, ok. And similarly the size of the box starts growing very large the energy levels become very very fine, ok.

So, let us so this is an important message as well. So, not only is not only the energy pretty reduced the energy spacing going to reduce with the mass of the particle, but if I were to increase the size of the box and you look at all these energy levels, you will find that the energy levels are much more closer to each other here, ok because once again the difference in 2 consecutive energy levels varies as 1 by L square.

So, if we think about the electron. So, how does this connect with our semiconductor physics? So, if you were to think about the electron, and let us say it sitting in some material, and it sitting inside of potential well which cannot resemble this box and in fact, there does exist such a potential well which is the nucleus of the atom. So, if you think about the nuclei it is got let us say positive charge and therefore, it is got a certain electrostatic potential and the only thing is its not shaped like a box, but the electron is in some sense held inside this potential well.

So, if you were to imagine all this as a box, and if you look at the amount the electron is allowed to move about around this nuclear, and if you sort of imagine an effective length or that effective size the box to be that then the energy levels electron can take, ok. So, in a material in which the electron is more or less free it is much more finely spaced as compared to an electron which is not so free, ok.

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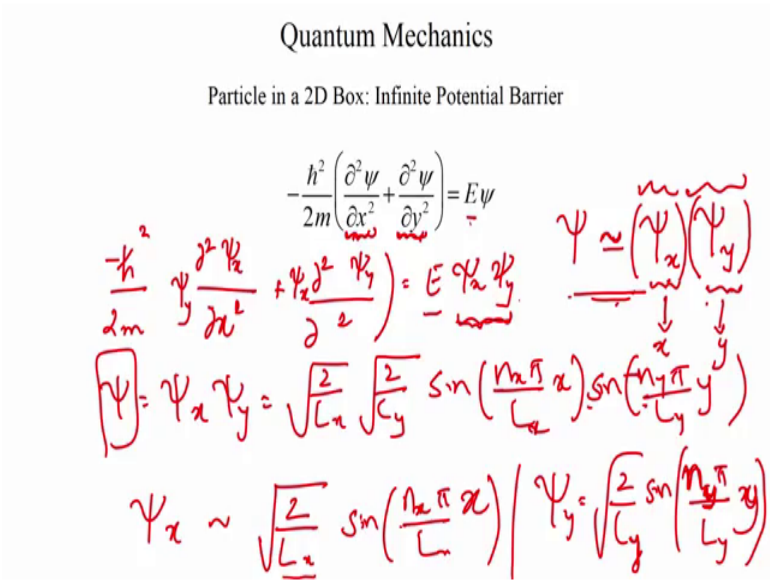

Now, let us sort of extend this idea, which sort of generalize this idea to a 2D case, ok. So, let us say the particle is not sitting inside a one dimensional box, but it is sitting inside a two dimensional box. And it will still retain the fact that the, you see the particle see is an infinite cliff, ok. So, you can sort of imagine a 2D box and for the time being I will draw a rectangular box, for mathematical convenience as I will show you.

So, let us imagine a rectangular box. So, it is a two dimensional drawing here it is a. So, on the on the z axis you have potential, ok, so let us call that y and let us call this x. So, initially we only looked at that as a 1D case, where the distance was only in one direction, but now, you have a two dimensional distance plane, ok. So, this could be L x, let us call the width the box next direction is L x and the width of the box in the y direction as L y, ok.

So, it goes from 0 to L y. So, I have to draw the coordinates this would be my coordinate system. So, that is L x comma 0, and that is 0 comma L y and this is 0 comma 0. So, let this be my coordinate system. So, I am only looking at the floor and if I were since it is A since my potential is on the y axis the potential of this floor of this box is 0 and the potential over here which is you know outside in the regions outside of this box, ok.

So, it is a hollow box and there is space all around it and that potential is infinitely tall, ok. So, this is infinitely high, these are all infinitely tall walls and there is this little hollow which is sitting at 0 potential and it is got a length x in the x direction L x in the x direction and length L y in the y direction. So, that is the situation I probably should have had a nice drawing here, but if you can if you can understand this drawing of mine you have this situation in place. So, we want to solve Schrodinger's equation for this case, ok.

Now, since I chose a nice little rectangular box I can use one simple trick which is I can say that my psi can be written as a product of two components, the psi in the x direction and the psi in the y direction, ok. So, let us say my psi my wave function for the particle can be written as a product of the wave function in the x direction and the product of the wave function in the y direction. So, if I were use this relation right here my Schrodinger's equation which now, has got 2 terms because you now, have to consider the potential the momentum in the x direction and the momentum in the y direction. So, it is got the x and y aspects to it and that is my total energy my potential is still 0, ok. So, it is just Schrodinger's equation, but written out in the 2D case and it is still the time independent Schrodinger equation.

Now, if I were to use this particular condition in my Schrodinger's equation I will end up with dou square psi x psi y by dou x square plus dou square psi x psi y by dou y square is equal to E psi x psi y, ok. Now, psi x is purely dependent on x and psi y is purely a function of y, ok. So, this is not a function of x and that is not a function of y, so which means that as far as this derivative is concerned psi y is just a constant coefficient, ok. So, you can put that outside your derivative and as far as this derivative is concerned psi x is a constant coefficient and you can place it outside, ok. So, that is my differential equation.

So, now let us mean let me divide throughout by psi x psi y, ok. Now, E is a constant coefficient and therefore, I end up with minus h square by 2 m and I am going to divide throughout by psi x psi y 1 by psi x dou square psi x by dou x square plus 1 by psi y dou square psi y by dou y square is equal to a constant which is energy, ok. So, if you look at this particular term here it is got 1 by psi x and its dou square psi x by dou x square there is no y component at all, there is no psi y, there is no y, ok. So, this parameter here is not at all influenced if you play around with the y aspects the wall box.

So, if I say increase or decrease L y this first term here should not be should not, it should not matter to this term at all. And similarly the second term here is purely a function of y only, and it should not matter to it as to what is happening in the x direction. And because this is the case I can rewrite my energy as having two components, one is the energy in the x and the other is the energy in the y. And I can split this in such a way that I can rewrite this one equation as two separate equations because I have got the same message, ok. I can write this as, this is the first term of your, this is the first term on the left hand side and that is equal to E x and let us say minus x square by 2 m 1 by psi y tau square psi y by dou y square is equal to E y. So, let us write this equation it split it into these two terms,

If I were to take this psi x to the other side, I end up with the equations looking that way I take the psi x and psi y to this side these are my equations. Now, these two are you are very familiar set of equations which you solve for the particle in a 1D box and therefore, you can solve these two Schrodinger's equations independently, ok. So, you can now, solve these two Schrodinger's equations independently and say that my psi x has got a function a wave function that the psi x looks very similar to what you saw before it should be of this form square root of 2 by L x sine of n x by L x pi by and L x into x. And psi y will be at the form square root of 2 by L y sine of n pi, pi by n y pi by L y into y, ok.

So, this is psi x it depends on the length of the box in the x direction and it depends on a quantum number or integer n x. And on this side you have the psi y depending on the length of the box in the y direction and another quantum number or an integer n y to satisfy all the boundary conditions. And the total wave function is simply the product of these two which can now, be written as psi x into psi y, ok.

So, the total wave function is psi x into psi y which is square root of 2 by L x square root of 2 by L y into the product of the 2 sinusoid terms, sine of n x pi by L into x sine of n y pi by L y into y. So, this is the solution or Schrodinger's equation in a two dimensional box, ok.

So, it was convenient for us to separate these two terms, ok. Now, that may not always be possible. So, for example, if you have, so here the coordinate system I chose it was a rectangular box, and in a rectangular box the x and y directions were orthogonal components. If you look at the basis vectors I have chosen 2 orthogonal components there. Now, if you had a box say it was shaped as a triangle probably not so obvious, ok. But nevertheless just to illustrate this point, I think this is a good message.