Semiconductor Devices and Circuits

Prof. Sanjiv Sambandan
Department of Instrumentation and Applied Physics
Indian Institute of Science, Bangalore

Lecture- 03
Quantum Mechanics: Particle in a Box – Continued, Harmonic Oscillator

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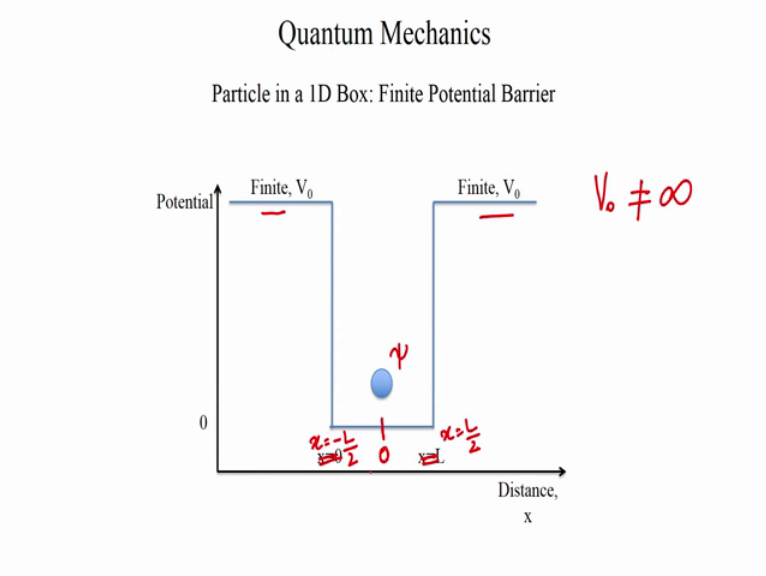

So, let us now consider the next case, which is the particle in a one-dimensional box, but instead of the potential being infinitely large you know outside this box, we will now lower the potential to a finite value. So, it is exactly the same kind of a diagram or you know kind of a potential profile, but the only big difference is that these potentials that you see here, where initially infinite, I have now made it finite, and it is got a value of V naught ok, and this is no longer infinity.

And you still have the particle, although I have drawn it as a discrete particle we should remember that it is actually a wave function. And for the sake of simplicity, let us actually define this box to be at minus x minus L by 2 and L by 2 ok, so that everything that happens is we will watch out for symmetry across x equal to 0 ok, so that is our that is our definition.

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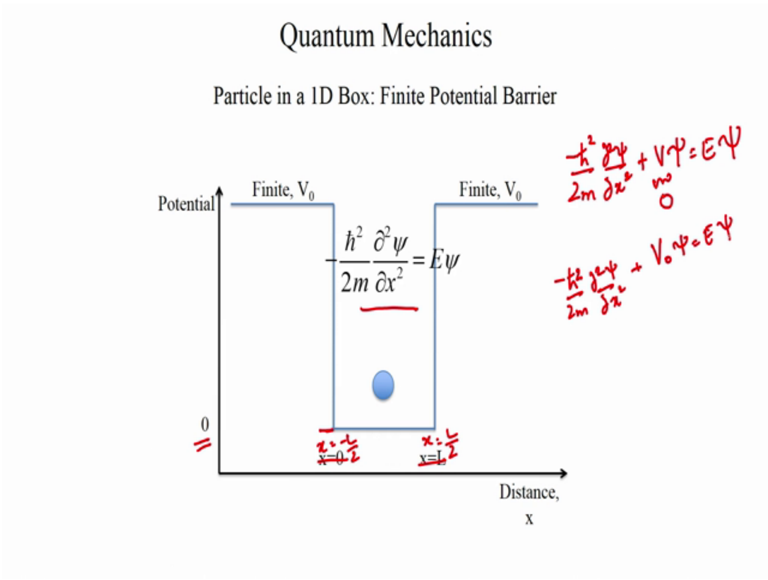

So, how do we write Schrodinger’s equation. Now, inside the box we firstly, let us let us write Schrodinger’s equation in a very general sense, so you have minus h bar square by 2 m dou square psi by dou x square plus V psi is equal to E psi. So, this is Schrodinger’s equation. And we always wanted to identify what this potential is and just like in our previous case inside the box, we can define the reference potential to be 0 ok. And once again let me correct these axis, because that sort of is consistent with what I have written later. And inside the box we find that Schrodinger’s equation is simply this, because my potential term is 0, because the potential is 0 inside this box.

Now, outside the box in the previous case, when we considered an infinitely high potential barrier, we had assumed that the wave function does not exist right. And if and we and we went ahead to only solve for the wave function inside the box, but now we can write Schrodinger’s equation outside the box. And you know using the same idea here, you will be able to write Schrodinger’s equation outside the box, and instead of the potential being arbitrary V, it is actually V naught, because that is the way we have defined our potential.

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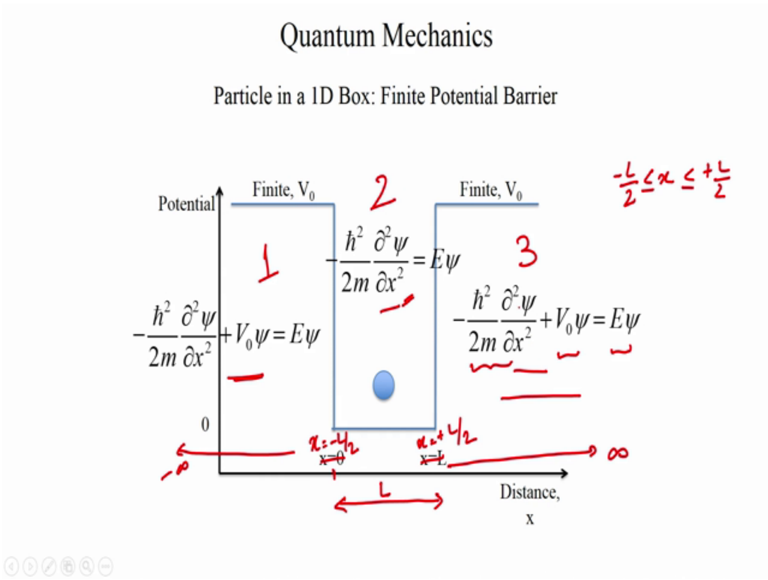

So, outside the box, the potentials would the Schrodinger's equation will take a form that look like this. So, you have a kinetic energy, you have a potential energy that is equal to the total energy. And inside the box, we have Schrodinger's equation taking a form like this. And we will define the coordinate system to be x equal to minus L by 2 x equal to plus L by 2 on the right side; therefore, the box still got a width of L. And from x equal to L by 2 all the way till infinite, you have this Schrodinger's equation; from x equal to minus L by 2 all the way down till minus infinite, you have this Schrodinger's equation.

And inside the box that is from for the region of minus L by 2 less than equal to x less than equal to plus L by 2, you have this Schrodinger's equation. So, I will call this as region 1; I call this as region 2; and call this as region 3. So, you have three different regions, and you have written Schrodinger's equation for each of these regions.

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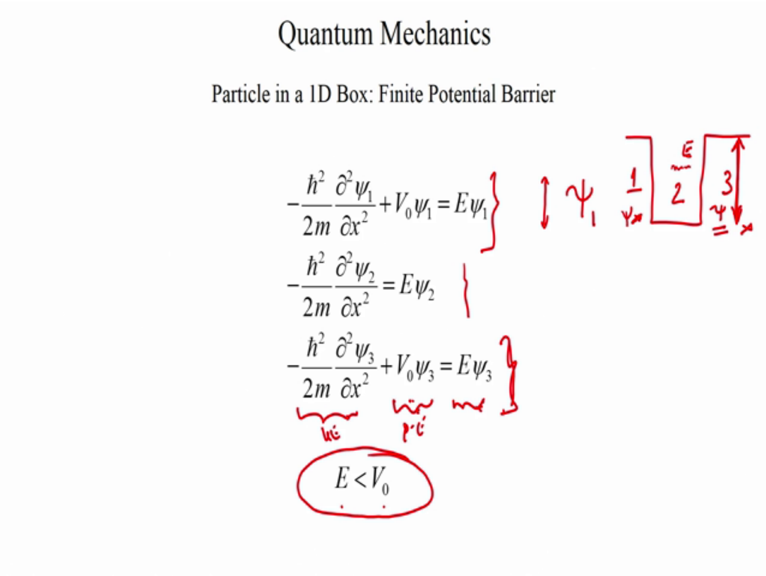

So, just to summarize, these are the three wave functions; we have psi 1 for region 1, and if I just draw the box here again, this is psi 1; and then we have psi 2 for region 2; and you have psi 3 for region 3. Now, the first point is that let us assume that E is less than V naught. Now, this seems to be a very difficult assumption to taken, if you observe this carefully. So, what are we saying here, by saying that E is less than V naught. What we are saying is that yes, the particle does exist somewhere, and it is got a total energy E, and that total energy E is less than the potential height in region 3. And we have still gone on to write Schrodinger's equation in the manner shown here ok.

So, what we are saying is, this is the kinetic energy; this is the potential energy; and the sum of the kinetic energy and potential energy is equal to the total energy, and that total energy term is less than V naught, which means the total energy is less than the potential energy ok. Now, that is that is that sounds a bit odd ok, but it is one of the main features of quantum mechanics. So, if E is less than V naught, and if the if I have to describe a wave function here in this region regions 1 and 3, then what I am trying to tell you is that the kinetic energy has got a negative value, that is that is that is the implication of it; I mean that is what it that is what classical mechanics would tell you.

In classical mechanics, if E was less than V naught, there is no way the particle can have an existence outside region 2 ok. But, what we are seeing here is that we are able to write the Schrodinger's equation, it does there is nothing to stop us from writing Schrodinger's equation, even outside the box ok. So, let us see where this leads us.

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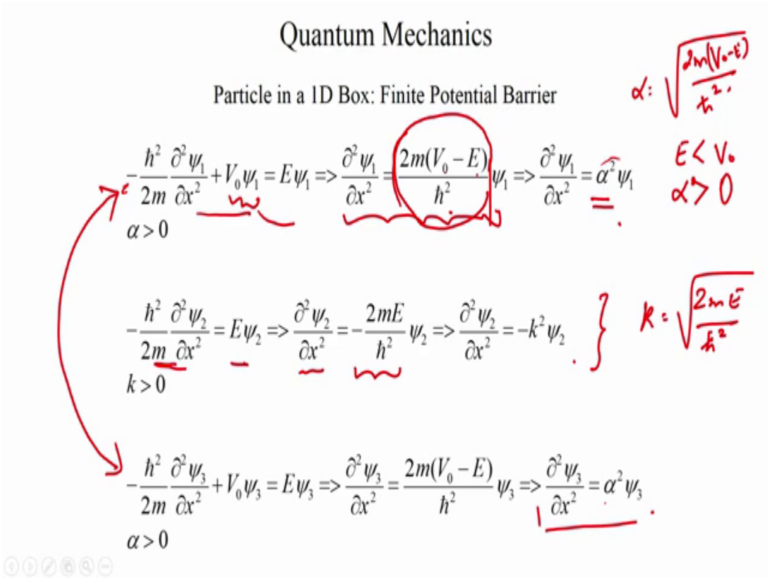

Now, firstly let us get some definitions clear ok. So, we have this to be our Schrodinger's equation, I am just going to take the V naught term pull it over to the right side and get rid of the negative sign here, and I am going to write the same equation in this manner. So, I have taken h bar squared down here 2 m has gone up there and this is V naught minus E; and therefore, the negative sign of this term has disappeared ok. And we will just call this entire term component here, this entire component here to be equal to alpha square.

So, since my E is less than V naught alpha square, I mean our alpha is greater than 1 greater than 0 sorry. And similarly, for the region for in region 2, we have Schrodinger's equation to be the kinetic energy is equal to the total energy. And I can rewrite this as dou square psi 2 by dou x square is equal to 2 m E by h bar square. And we will define this term here as minus k square ok. Now, this is this is a this is a situation that is similar to what we have done before, the only thing is I am trying to bring in consistency between the way we represent these equations ok.

So, we have minus k square, where k again is greater than 0. So, my k will be square root of 2 m E by h bar h bar square, so that is my k. And in this case, my alpha is square root of 2 m V naught minus E by h bar square. Similarly, for region 3 we write Schrodinger's equation in a manner, which is quite similar to region 1 ok. So, once again we define the alpha is the same, so we have Schrodinger's equation and region 3 to be this, so that is region 1, that is region 2, and this is a region 3. Now, the big difference between region 1 and region 2 is that here alpha is positive, and this entire term is positive, but here since k is also positive, there is a negative sign here, and therefore this entire term is negative ok, so that is that is the big difference. And once again in region 3, you have a positive term on the right hand side.

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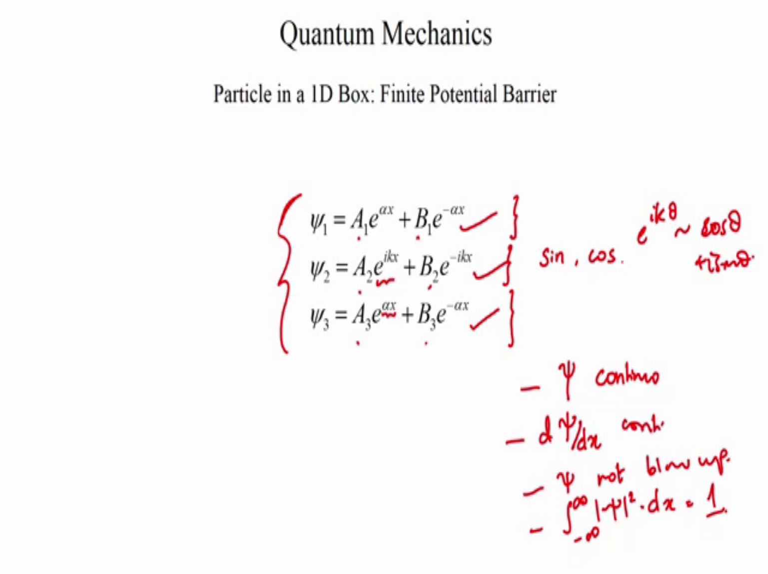

So, since I have Schrodinger's equation in that particular manner, I can write an expected solution for the wave function. So, as I mentioned in this region the right hand side term is positive ok, and we need to guess the solution for say psi 1, so that when you take the second derivative, you end up with a form that is got psi 1 in it, and it is also got a positive term. And that solution could be of this form ok; it will have you have exponentials of a real number, then you will end up with a possible solution for that.

Similarly, in region 3, you have a similar description, where you have exponentials of a real term. But, in region 2, we already saw that you know you could describe things as sines and cosines, when we solved when we solve Schrodinger's equation for this equivalence of region 2 in the infinite potential well case; we saw the sines and cosines appearing in the equation.

And equivalently you have if you write it in terms of exponents, you are going to have exponents of complex quantities that are appearing in region 2. So, and you know by Euler's notation, you have this being equivalent to your equivalent to your sines and cosines. So, these are the three general solutions that are possible. So, phi 1 is expected to look like that, psi 2 is expected to look like that, and psi 3 is expected to look like this.

Now, how many terms do we need to identify, we need identify A 1, B 1, A 2, B 2, A 3 and B 3 ok. And what are the properties that we have, we have that firstly, psi has to be a solution Schrodinger's equation that is all satisfied by defining psi in this particular manner; that we must have psi to be continuous, you must have d psi by d x also to be continuous, and you must have psi not blow up, it should be normalizable, it should not blow up anywhere.

And basically equivalent to this condition is also the other side of it, which is that psi the way the particle must exist somewhere. And therefore, in this space from minus infinite to infinite, the particle must exist somewhere, therefore the probability of finding the particle in some region there is 1 ok. So, we have all these terms to play with.

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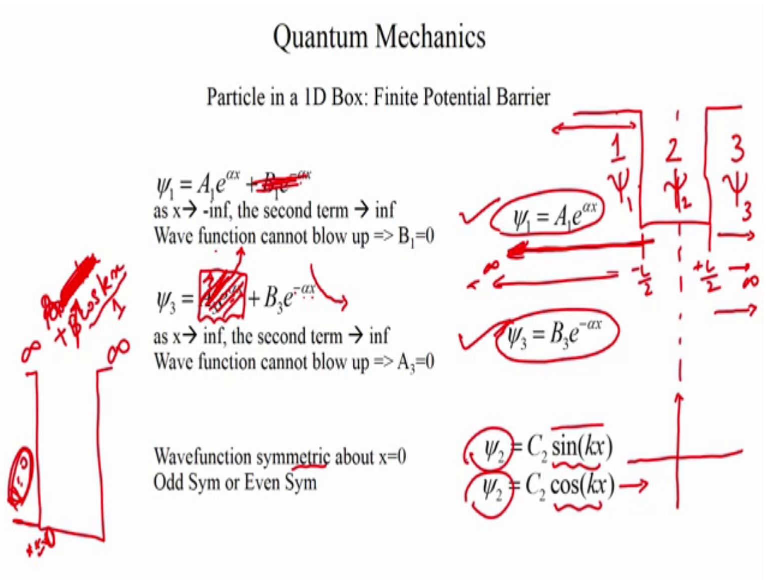

Now, let us just go through the process of elimination, and trying to bring out some useful results here. So, first let us take the region 1 ok. So, let me redraw the box here, so that was my region 1, that is region 2, and that is region 3. And for regions mentioned before, this is the general solution for the wave function in region 1; this is the solution for the wave function in region 3; and for region 2, you have sins and cosines ok. Now, let us take region 1 first ok. So, let us let us not worry about region 2 and 3, let us just take region 1, which is this region.

Now, let us imagine, since the general solution, let us start seeing what happens to solution. If I start moving towards minus infinity I start walking in this direction and go from x equal to minus L by 2 to minus infinity ok. At x equal to minus infinity, so as we start moving in the direction what happens to this term, now alpha is positive. So, as x starts getting more and more negative, this term starts dying out.

What happens to the second term? Since alpha is positive, and x is negative, this negative sign disappears, it becomes a positive value here. So, you have e to the power a positive quantity, and that positive number starts increasing as I head towards x equal to minus infinity. So, this term starts increasing, as we head towards minus infinity. Now, we already mentioned that the wave you cannot have any of these components blowing up, which means you cannot have them head towards infinite. And since, this is doing exactly that in region 3 in region 1, as I move towards minus infinite, this term cannot exist you cannot allow this, this might be a general solution, but this term violates this very basic principle that you cannot have the wave function blow up ok. Therefore, the B 1 term has to be 0 ok.

And if B 1 is 0, I can just write my solution to be just this, psi 1 is equal to A 1 A to the power alpha x, so that just by a process of simple you know by just using simple arguments, you have eliminated one of the coefficients, you do not have to identify that. Now, what about region 3 and you can make the same argument here, but the only thing is that region 3 exists from plus L by 2 all the way till infinite. So, if you start moving towards plus infinite ok, you cannot head towards minus infinite, because that is not region 3 ok. So, psi 3 is not valid for, if you are heading towards minus infinity. So, as you head towards plus infinite, what happens to these terms, alpha is positive, and you are heading towards plus infinite. Therefore, this term starts blowing up.

Now, here you have a negative sign, and alpha is positive, and you are increasing x from L by 2 to infinite, therefore this term starts dying out ok. And since, once again since you cannot allow the way function to blow up, this component cannot exist you cannot allow that. Therefore, in region 3, the wave function must take a nature that looks like this. Now, in region 2, you could have sines or you could have cosines.

Now, in the case of an infinite potential well, if you remember the infinite potential well ok, where may had a solution a general solution of I think we used A and B there, A sin k x and B cos k x, when we had this general solution. At this at the point of x equal to 0, when we apply the continuity of the wave function at x equal to 0. Sin of k at x k x at x equal to 0 was not non-existent, but the cosine term became 1. And therefore, the term B had to disappear, because the wave function had taken a value of 0 outside the box, so that was if you just recollect the infinite potential well case that is what happened, so the cosine never existed in that case. But such a boundary condition need not happen now, because psi need not be equal to 0. So, you could have the cosine term surviving, because there is no condition for you know the wave function to be 0, when x is 0 for example ok, there is no enforcing condition. So, you could have both these cases.

So, if that is the situation, and we only look about look at symmetric solutions of the wave function so, we will look at solutions that are sort of symmetric around this midpoint. So, you could have psi taking a sinusoidal expression or it could have a co sinusoidal expression. So, this would mean that the wave function is even ok. So, it is got the same sign on both sides of the symmetry and this would mean that the wave function is odd, it is good find changes as you cross the symmetry. So, we can look at both these solutions; so you have psi 1, you have psi 3, and you have psi 2, which could be either this or that for the purpose of symmetry.

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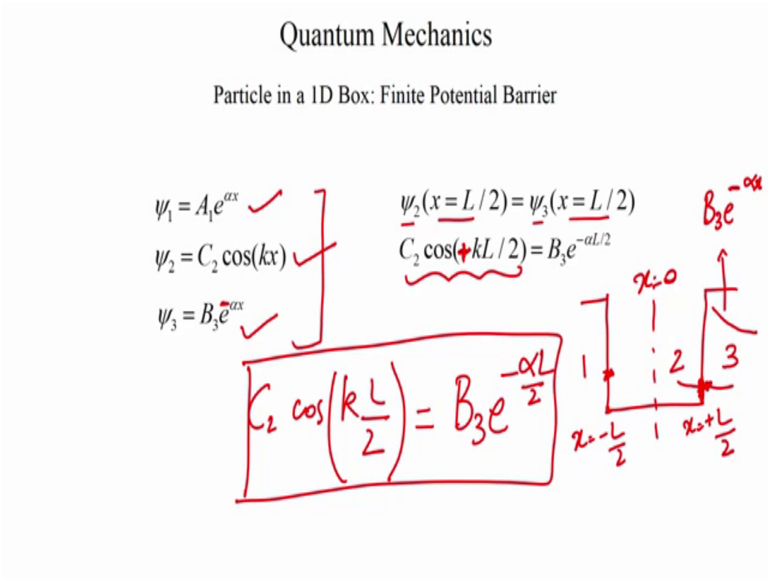

So, let us go through an example of having these three cases; so that is my psi 1, that is my psi 3 and let us say we are looking at even wave functions in region 2. And let us say that is my wave function in region 2. So, firstly, how do we identify all these terms ok, now the first thing we do is let us say the wave function is continuous. So, the wave function you have the box here, this was x equal to minus L by 2, that was x equal to plus L by 2, and that is x equal to 0, now this is region 2, that is region 3, and that is region 1.

Now, if you look at this boundary here, since the wave function has to be continuous, psi of psi 2 at this point must be equal to psi 3 at this point ok. So, psi 2 at x equal to L by 2 must be equal to psi 3 at x equal to L by 2 ok. Now, what is psi 2 at x equal to l by 2, you have C 2 cosine k L by 2 that is my psi 2 ok. So, this is a typo, please pardon me; there should be a plus here, so that is that is psi 2. And what a psi 3, psi 3 is given by phi 3 is given by B 3 e to the power minus alpha x ok. So, we saw that only the decaying term is allowed here, so it is B 3 e to the power minus alpha x that is my psi 3. And once again there is a typo there should be a minus sign.

And therefore, at x equal to L by 2, phi 3 takes a value of L by 2 e to the power minus alpha L by 2. So, this is the first condition, which is simply the continuity at L by 2. Now, since we are looking at symmetric cases, there is not you are not going to learn too much by applying the same continuity at minus L by 2 ok, so that is not going to give you too much of new information. But, we have you know whatever solution holds here, you could just directly apply the solution on the other side just taking into consideration the direction in which we move. So, this is the first condition.

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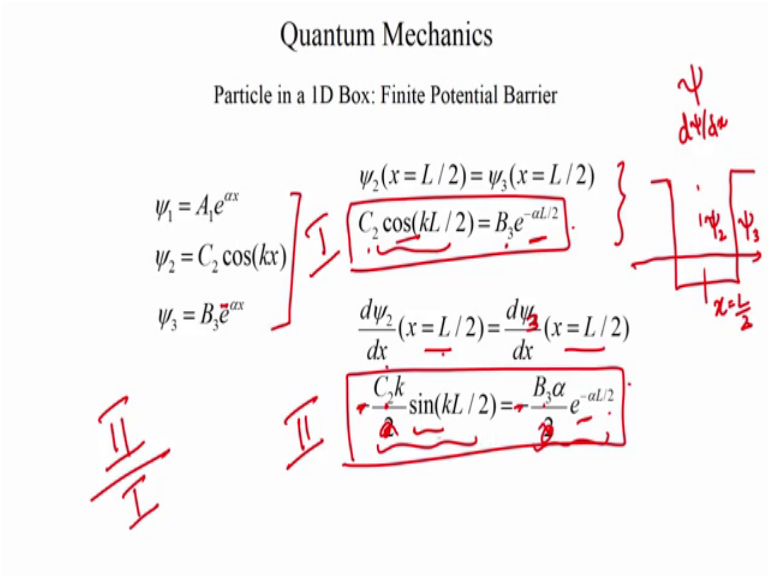

Now, what is the second condition? So, we have these three solutions; we have the second condition, this is the continuity you know constraint, but this first derivative of the wave functions to also be continuous right. So, if I have x equal to L by 2 here, I must also have not only psi being continuous, but I also need d psi by d x to be continuous. Now, since the wave function has got a form psi 2 in this region, and it is got psi 3 here, I need d psi 2 by d x at x equal to L by 2 must be equal to d psi 3 by d x at x equal to L by 2. So, the first derivative of the cosine is going to be minus it is going to yield minus C 2 k by 2 sin of k L by 2, and this is going to yield this term all right.

So, you now have this condition, and you have this condition. And now, you can go ahead and apply the condition that the probability of finding the particle somewhere in all 3 regions has to be 1. But, let us not head there, because let us just investigate what is needs to be investigated this point, because those details do not really serve our purpose too much. So, what we are going to do is just examine these two terms. Now, you see this you have a sinusoid, you have a co sinusoid, you have C 2, C 2 and you have B 3, B 3, and you have the same kind of an exponential term.

So, suppose I were to label this equation as equation 2, and this is the equation 1, what I would like to do is take divide equation 2 by equation 1. So, you will have the negative signs have already gone here, the 2 will disappear.

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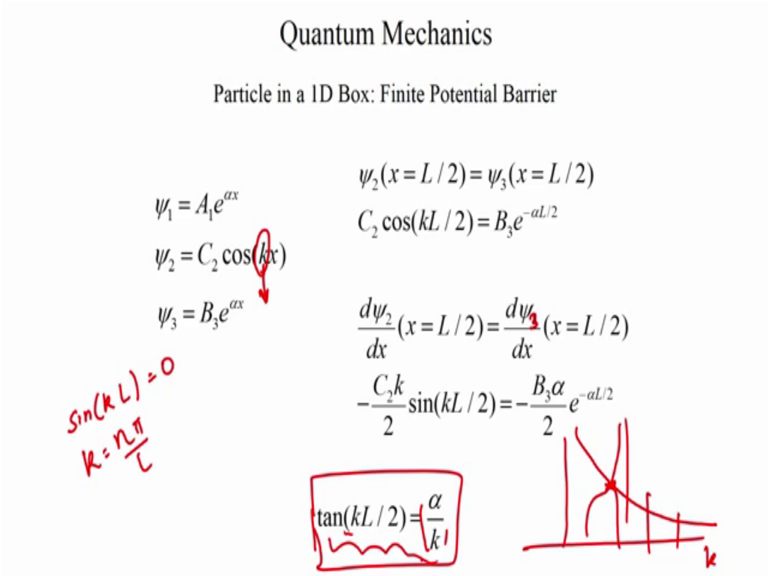

And, if you were to divide this term by that term, then you will end up with the condition that the tangent of k L by 2 is equal to alpha by k. Now, k is an important parameter for us, because you have k defining the wave number in some sense. Now, if you ask yourself the question, in the case of an infinite potential well, what were the values k took. So, in that case you had to meet the condition that k L was equal to 0, and therefore k could take integer values of pi by L.

Now, in this particular case for a finite potential well, k can only take those values, where this equation is satisfied ok. So, if you were to plot if you were to plot both these functions ok, let us plot alpha by k (Refer Time: 23:59) how does alpha by k vary with k ok, it would probably vary in this manner. And then, you plot how tangent of k L by 2 varies with k ok, you will get another plot.

And if you were to take if you were to take the points at which these two functions meet, those are the values of k that are those are the solutions of solutions of these particular equations. And only those values of k are allowed; so no other values of k are allowed. And then, you could use this k to define your energy, so that is the first point.

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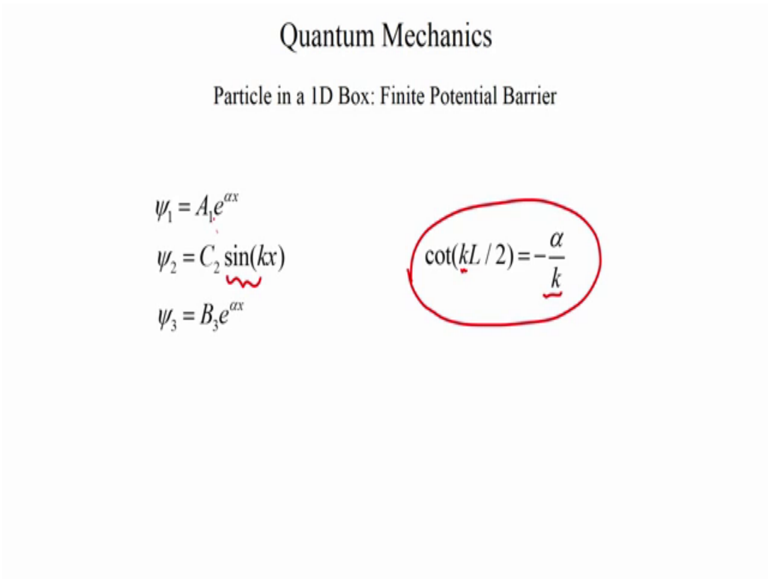

Now, the second point is if you consider the odd symmetric case that a side to being C 2 sin of a k of k x. You will end up with the condition that the cotangent of k L by 2 must be equal to minus alpha by k. So, once again k can take only those values that are permitted by the solution to this equation. So, as I mentioned it really does not serve our purpose too much to spend a lot of time calculating the exact values of A 1, C 2 and B 3.

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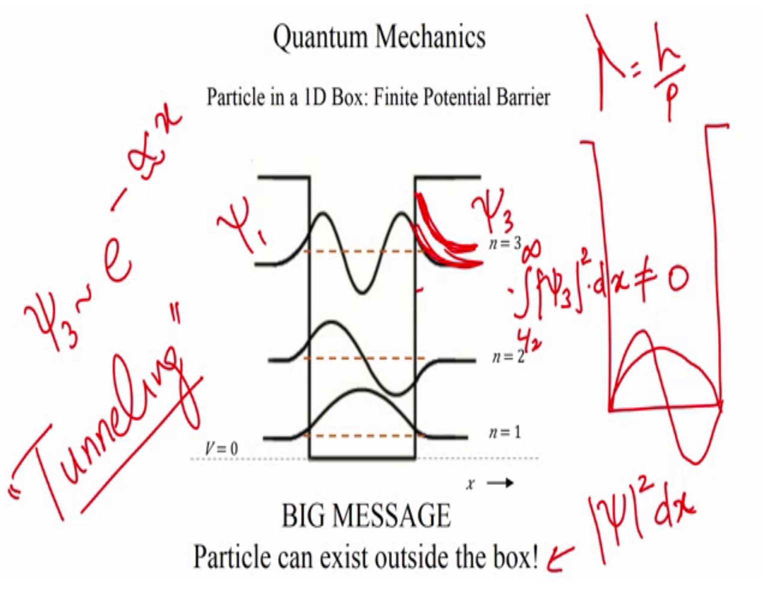

But, what is useful to note is that the solutions will have the wave functions will sort of look like this. So, we have sort of sketched the wave functions here. So, in the case of an infinite potential well, the wave function existed only inside the box. So, we found solutions like you know if the wave function is to be like this. Now, in the case of a finite potential barrier, we have already seen that psi 1 and psi 3 can have an exponential solution. So, if you look at psi 3, it varies as e to the power minus alpha x with alpha being a positive number, so which means the wave function has got a decay in space in the x direction.

Now, mathematically that looks fine ok, it is not does not seem to be very difficult, because the exponential came out from the differential equation. But, just imagine what it is implying, you have a finite potential barrier ok, and you have got the total energy of the particle to be less than the potential energy of the barrier ok.

So, class according to classical mechanics, the particle can never climb over the barrier, but what quantum mechanics is telling you is that by solving Schrodinger's equation, we are finding that the wave function exists outside this well, and it exists by decaying exponentially with the distance ok. So, the wave function exists, and it decays exponentially with the distance, so that is a very big message. What quantum mechanics is telling you, is even though e is less than the height of the barrier, the particle can exist in that region ok.

So, if you imagine if you remember, psi is indicative of phi square is indicate with the probability density function to find or finding the particle in any given regions. So, size square d x is the probability of finding the particle between x and x plus d x. The probability of finding the particle between x equal to L by 2 and infinite is now given by psi 3 square d x L by 2 to infinite. And what quantum mechanics is telling you is that this probability is not 0, even though the total energy of the particle is less than V naught ok. Now, that is a very amazing result, if you think about it ok, but it is so naturally seen if you simply solve Schrodinger's equation.

But, this result is important; and it is in fact, used on a day to day basis, it is not that it is a interesting exotic result that has got no implication. Now, if the particle for example, if the particle could not exist in this region, many of the devices if you are a since we are talking about a semiconductor device course, many of the devices and instruments that you use probably would not work. For example, the injection of carriers at the source drain, the source drain regions are doped, so as to encourage the injection of carriers through a mechanism like this you know in a MOSFET.

If you have heard of the something called as a scanning tunnelling microscope, that do works on the principle of trying to measure the electrons that are that have escaped the well and are found inside a barrier ok. So, this mechanism of finding of getting the particles to go through the barrier, if you may imagine the wave function is going through the barrier ok, despite the fact that e is less than V naught. This mechanism is something called as tunnelling ok; it is a technical term, but if anyone sees the word tunnelling, this is what they are talking about ok. So, this is what they need to think about, so that is a very important message of quantum mechanics.

So, if you have to summarize two important things, we have learned so far. The first is that particles also have a wave, and that wave length is given by the De Broglie's equation lambda is equal to h by p. And the second is the fact that the wave function can exist outside a barrier, even though the total energy is less than V naught. So, these are two important essential points.

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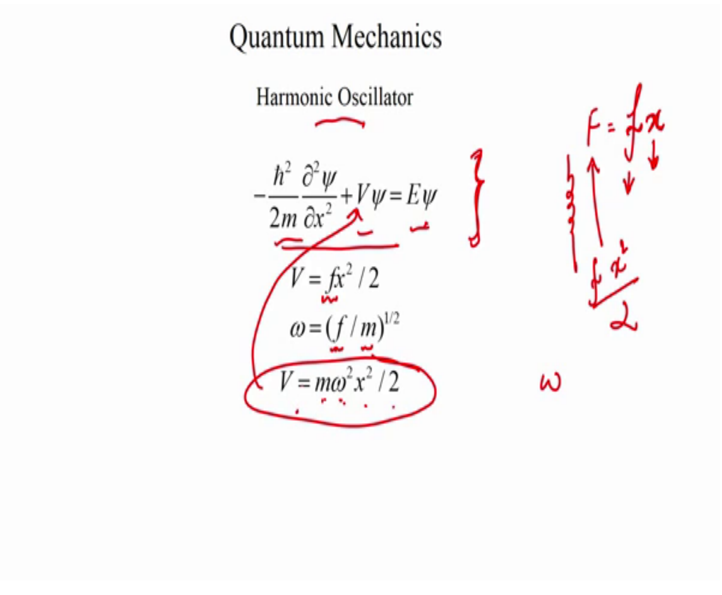

Now, before we wrap up quantum mechanics the topic, let us just quickly go through another example of using Schrodinger's equation. And this is an example of something called as a harmonic oscillator so, we want to see you know what is the nature of the wave function here. So, let us write down Schrodinger's equation for in a very general sense, so that is the kinetic energy, that is the potential energy, that is total energy.

And since, we are talking about an oscillator I think the easiest way to imagine one is to imagine the equations for a spring ok. So, if you remember, the spring if you apply a certain force to a spring, then it is got a certain spring constant ok, which I have when I have used a symbol F for it. But, in textbooks you might probably see the symbol k it is just that we are using k too many times. So, let us say F is the spring constant, then the force will be given by the spring constant times the displacement (Refer Time: 30:53) so that is. So, you can imagine you can imagine a little spring a quantum spring if you mean that we are trying to describe here, now that is the spring constant.

And the potential energy stored in a spring is f x square by 2 that is half the spring constant into x square, where x is the displacement. And if I were to let the spring go and oscillate, it would have a natural oscillation frequency of omega, which is equal to the spring constant divided by the mass per unit length, I am sorry at the mass to the power half. And the potential energy term would be can be rewritten by writing f in terms of omega and m as m omega square x square by 2, so that is my potential energy term ok.

So, with this introduction, let us just use this term for the potential term in my harmonic oscillator ok, so that is Schrodinger's equation and that is V, e is a constant, and that is the kinetic energy. So, that would allow us to write Schrodinger's equation in this particular manner.

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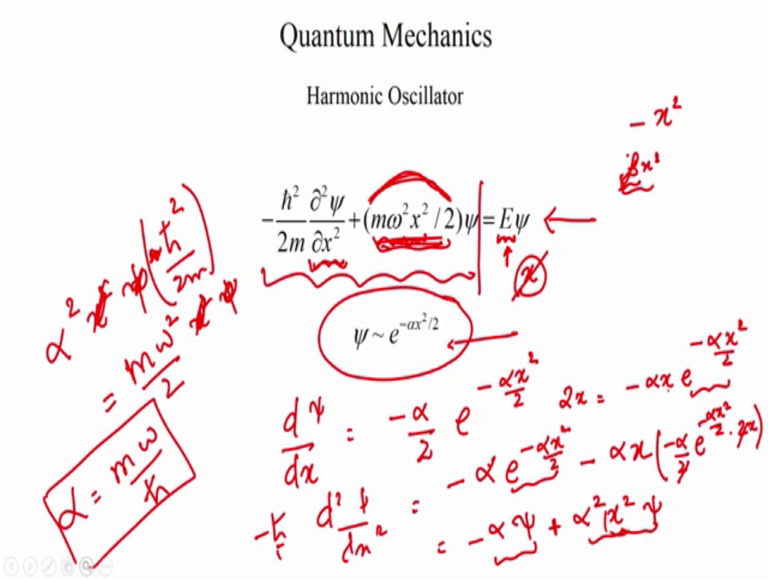

Now, how do we solve this? Ok. Now, this equation seems to be a little bit more complicated, then the ones you encountered in the case of a particle in a box ok. So, how do we go about solving this? So, we make a good guess that is usually the case for many situations, we make a good guess. And our guess is psi is equal to e to the power minus alpha x square by 2 and why is this going to be our guess? If you think about it the right hand side, here has got a e that is a constant that is a constant here, there is no dependence on x, there is no x at all on the right hand side. But, on the left hand side, you have a dependence on x here, and you have a dependence on x in this term.

So, somewhere by solving all this out, that x dependence must cancel off ok and what is the x dependence, it is very obvious that you have a factor that is multiplied by x square sitting here. So, I cannot allow that to exist after I have taken the derivative and cancelled all the terms, this term cannot exist ok, because otherwise if it dot if it did exist, then I do not see an x square on this side, and therefore it is not a correct solution. So, this term cannot exist.

So, what is the side that I could use, so that if I take a second derivative, it would end up with square a term which has an x square in it some say some factor beta into x square, such that beta would be equal to m omega square by 2, and therefore cancel off with the potential term here ok. So, the idea is to get eliminate x square from this picture and this seems to be a good guess for that, because, what does d psi by d x, d psi by d x is minus alpha by 2 e to the power minus alpha x square by 2, and then you take the derivative of the x squared term which is 2 x, so this is nothing but minus alpha x e to the power minus alpha x square by 2.

What is d square psi by d x square, d square psi by d x square is minus see you first take the differential of the x, so its minus alpha e to the power minus alpha x square by 2 minus alpha x and you again differentiate this term once more, and you will end up with minus alpha by 2 e to the power minus alpha x square by 2 into 2 x. So, this is going to be a minus alpha so, let us call this psi, because that is what are wave function is. So, it will be minus and you have you have a minus and minus here that will end up being a plus alpha square, these two terms would cancel off x square psi.

So, you see that you have a constant times psi, and you have something which is got an x square component in it and going by argument, this component should cancel off that component ok. So, for me to have all this work out, we need alpha square x square psi into minus h bar square by 2 m ok, so minus h square by 2 m must be equal to this particular term must be equal to your m omega square by 2. So, we do not need to create in the negative, because it is going to that is the opposite sign it for you to cancel so, the magnitudes of these two needs to be the same.

So, this m omega square x square by 2. So, this implies that my alpha so, these also got a psi here so, pardon me. So, this implies that my alpha is going to be m omega by h bar, so that is my alpha ok.

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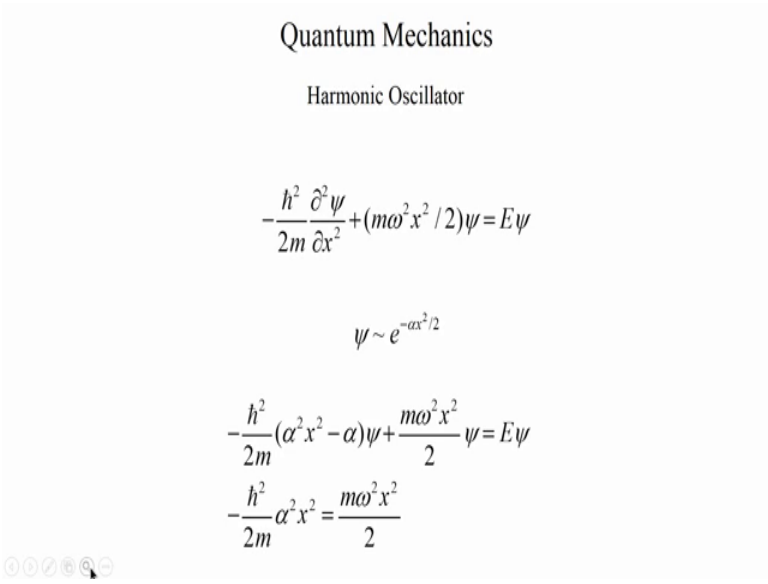

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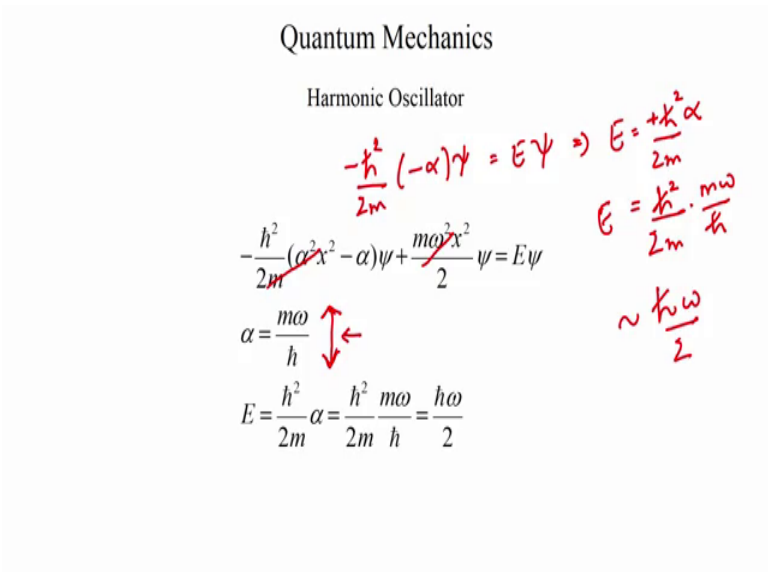

So, here is all this written out quite neatly. So, I need these two terms to be equal, and therefore my alpha has to be m omega by h bar. If alpha is equal to m omega by h bar, then I can now use this particular value of alpha to calculate what my e is ok. Now, these two terms have cancelled off. So, what is left is, on the left hand side is minus h square by 2 m into minus alpha psi is equal to E psi, implies my energy is minus h bar square by 2 m into minus alpha, which is h bar square by 2 m into alpha. And that using the value of alpha, you have h bar square by 2 m into m omega by h bar is my total energy, and which is going to be equivalent to your h bar omega by 2.

Now, what we have done here is we have only looked at the so-called ground state energy. So, it is not a very general solution to Schrodinger's equation. We just assumed one particular solution, you could have it could have had constant coefficients for example, but there are much that solution could be represent a much more general way, and we have not done that here. But, through these simple arguments, we saw the nature of the solution, which is the which is that the wave function must have a exponential of minus alpha x square by 2 component ok, so that is the nature of the wave function. And we found that the energy scales as h bar omega by 2 ok, now this is a very useful relation, which we will come back to later on.