Select/Special Topics in 'Theory of Atomic Collisions and Spectroscopy'

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Lecture 37

Scattering at High Energy

Greetings, we will continue our discussion on the behaviour of Phase shifts for large Orbital Angular Momentum, Quantum number L and examine how the phase shift changes with energy and momentum. And then, we will discuss other consequences of this situation. Now, we already obtained in our previous class.

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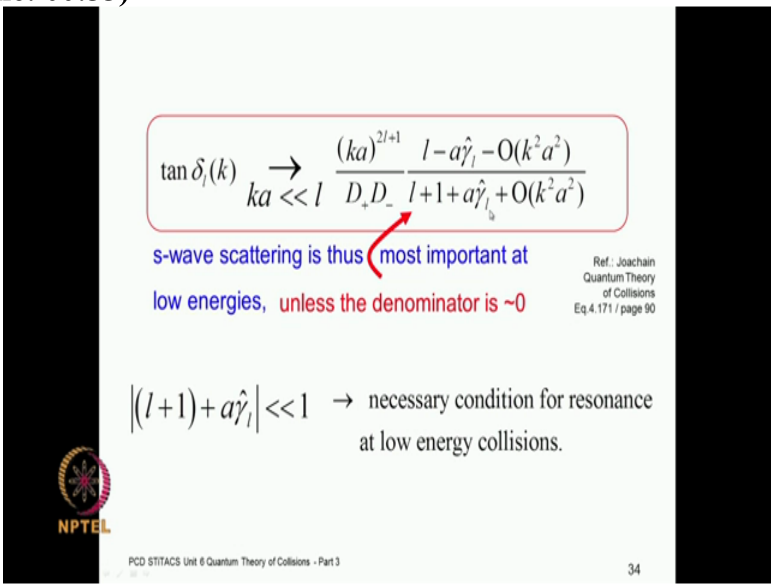

The expression for the tangent of the phase shift and we found that the resonance condition is given by this denominator going to 0; this l + 1 + a gamma. This gamma caret is the limiting value of the logarithmic derivative as k tends to 0, right. So, typically, because of this ka to the power 2l +1, all the contributions from higher orbital angular momentum will become less significant.

So, we have the expression for the tangent of the phase shift. And because of this k to the power 2l + 1, the contributions of higher orbital angular momentum partial waves will become insignificant unless, the denominator l + 1 + a gamma approaches 0. So, this becomes your necessary condition for resonance.

And we will have to examine, if s wave scattering is the only important contributor or are they are we going to expect some contributions from some of the other partial waves. And this is the resonance condition that we should examine closely. So that is what we are going to do now.

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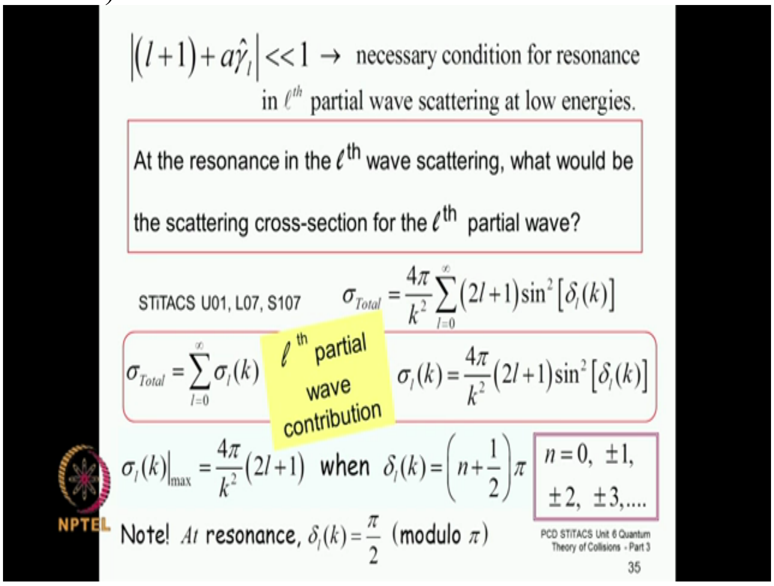

So, this is the necessary condition for resonance and the question is, if you do hit the resonance, if this denominator really becomes small, then, what will be the scattering cross section? What will be its contribution to scattering from the lth partial wave? So, we already know that the total cross section, you can write as a sum of partial wave cross sections from different orbital angular momentum quantum numbers, right.

So, you sum over all the values of l going from 0 through infinity and the lth partial wave is just 4 pi over k square 2l + 1. And then, you have the sine square of the phase shift for that particular partial wave. So, that is the contribution from the lth partial wave. So, this condition you can see will hit a maximum when the sine square function becomes 1, okay.

That is the maximum value it can take. And at that maximum value when sine square phase shift is equal to 1 the phase shift will be either half or 3 by 2 and so on. So, it will be n + half times pi. So, that will be the phase shift at this maximum. So, at the resonance the phase shift will be pi by 2 modulo 1. It can be pi by 2, it can be 3 pi by 2, 5 pi by 2 and so on. So, that is the resonance condition which we have.

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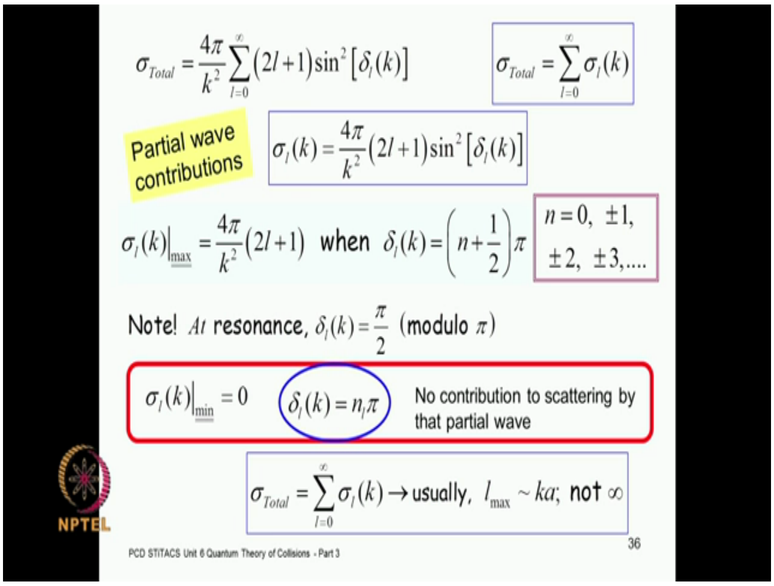

And the minimum value of course will be 0 when the phase shift will become npi. And there is no contribution to scattering by this particular partial wave in that situation. So, actually, although the expression requires for completeness that we must sum over, all the partial waves from 0, through infinity. But you really do not have to go to very large numbers so far as the angular momentum quantum number is concerned.

Because if you have a potential with a finite range then even from classical mechanics means. This is a semi-classical argument it is not very rigorous; but it works and it gives you at least an order of magnitude estimate of the maximum number of partial waves that need to be considered in the scattering phenomena; because r cross p with the angular momentum.

So, if you have a scattering target over here. And you have got a beam which is coming here, right. So, if this beam happens to become, come not just ahead on, but little above it so that there is an impact parameter corresponding to the range of the potential. Then, you can see that the r cross p, at this point, will give you an estimate of the angular momentum, right.

So, that is r into p, right. r into m into V and that will have to be the angular momentum. So, the Angular momentum, of course, is quantized. So, the Eigen value that you are really considering r Eigen values of l square which will, which will be h cross square l into l + 1. But you can approximate that for large value of l, l into l + 1 will be almost l. It will be almost l square and you can ignore the one compared to that.

Square root will give you well itself. So, h cross l will become of the order of r into h cross k. So, that tells you that the maximum value of the orbital angular momentum quantum number. That you need to consider will be of the order of ka and it will not really be infinity. So, you do not have to go to, you know, very large numbers in most of the physical situations.

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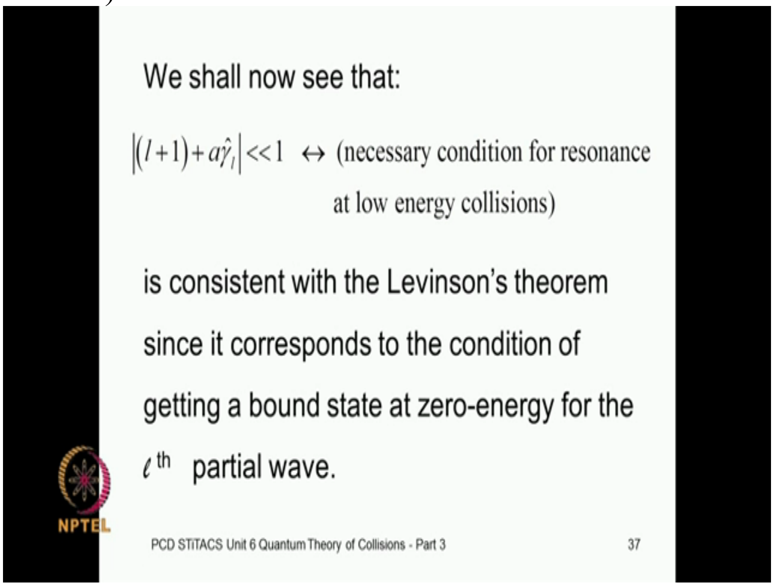

Now what we are going to discover, by doing a small exercise is that, this particular condition, which we have recognized to be the necessary condition for resonance, is completely consistent with the Levinson's theorem it, because it corresponds to the condition of getting a bound state for zero energy for the lth partial wave.

So, that is something that we would expect. And that is what it indeed turns out to be. So, we have to examine what is the condition to get a bound state at zero energy in the lth partial wave.

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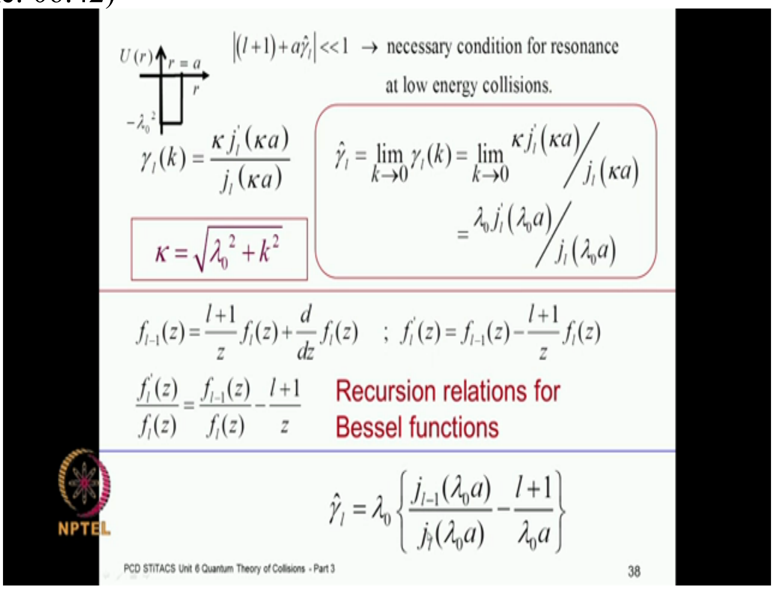

So, we do this again by considering a square well potential which is our prototype of a potential. The most of the other potentials are more complex but this example does illustrate the key ideas which go into this analysis. Now, for this square well potential, we have the usual dynamics over here.

The continuity of the wave function and is derivative is indicated by this logarithmic derivative gamma. And this is in terms of the Bessel function and its derivative. The argument of which is Kappa a, and Kappa is determined by the depth of the potential which is minus lambda 0 square.

And it is also determined by the energy which is k square, which is h cross square k square by 2m, right. So, this is the limiting value which goes in the necessary condition the gamma caret or the gamma hat is the limiting value as k tends to 0. So, as k tends to 0, so this term k square would vanish. And Kappa will be lambda 0. So, that is what you get in the limiting value.

What we will do is, to make use of the recursion relations for Bessel functions which you will find in Abramovitz and Stegun or even in Arfken or you know in almost any usual book on mathematical physics. You will find the recursion relations for Bessel functions and these are the standard recursion relations for Bessel functions, in which, the derivatives are given in terms of the adjacent Bessel functions okay.

So, there are similar relations for the normal functions and so on. So, you know this is the particular one for the Bessel functions. So, we make use of the recursion relations for the Bessel functions and then plug it over here to get the expression for the limiting value of the logarithmic derivative gamma in terms of the Bessel function for l - 1 and l.

So, these are the Bessel functions which appear in this because in the recursion relations, the adjacent values of l, they get connected along with the derivatives.
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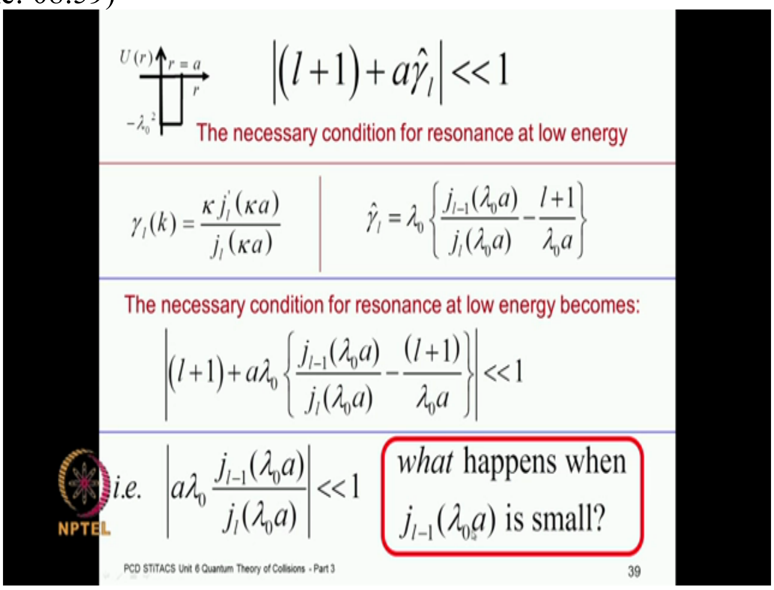

So we have this, using the recursion relation this form for the limiting value. And that gives us for the necessary condition for resonance. Now, in this a gamma, caret, we put the right-hand side from here, which we have obtained using the Recursion relation. And you have a times, this is a and then gamma caret which is this beautiful bracket multiplied by lambda 0. So, lambda 0 is here and the other beautiful bracket is here.

So, now you have got a lambda 0, here and a lambda 0, in the denominator. So, you can multiply both of these terms by a lambda 0. What happens when you multiply this a lambda 0? This cancels this. And you will have l + 1 here; and then, minus of l + 1 here. So those will cancel each other. And you are left with a lambda 0 times this ratio.

This product must be of absolute value which should be a small number okay. So, that is now effectively the necessary condition for resonance at low energy okay. So, now we ask what happens when this denominator is small.

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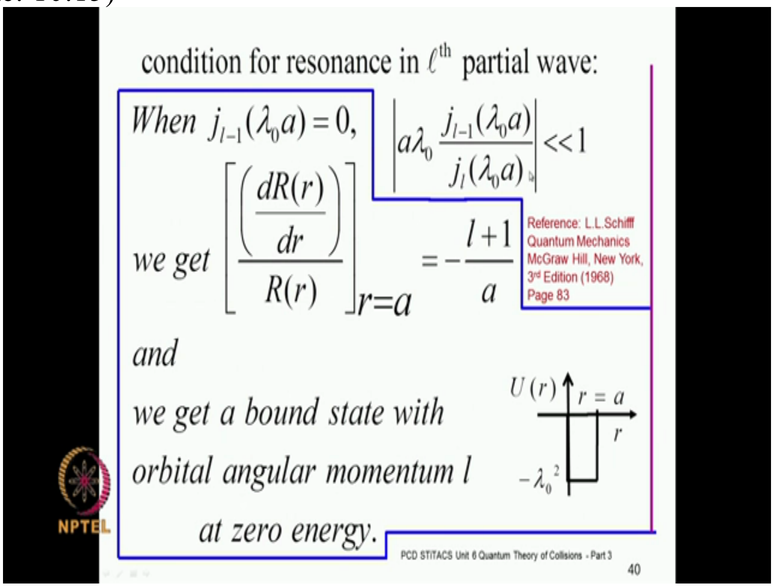

So, what is going to happen is that when this denominator is small then you get if you go through this exercise in Schiff's Quantum Mechanics which I will not work out. Then, you find that you get a condition for having a bound state.

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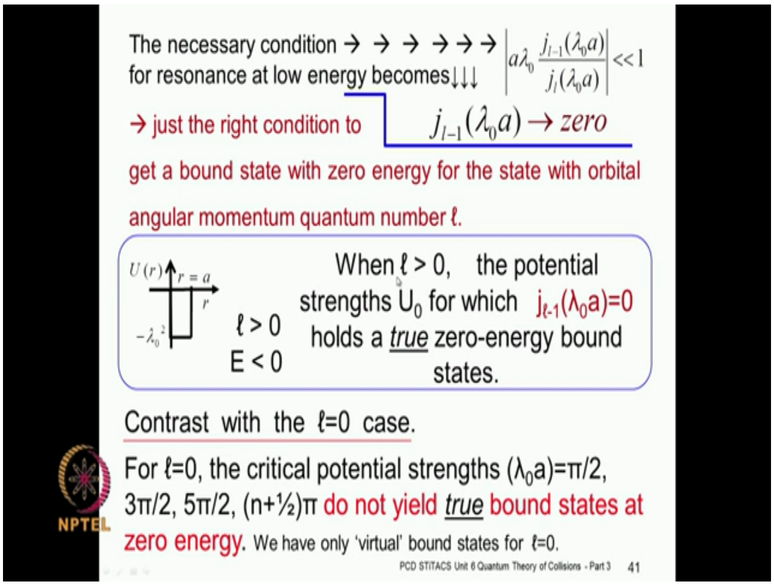

So essentially what is going to happen is that the condition that, that you get a bound state for l becomes completely equivalent to the necessary condition for resonance which is just the right kind of condition. The only difference between this and the case for the partial wave for l = 0.

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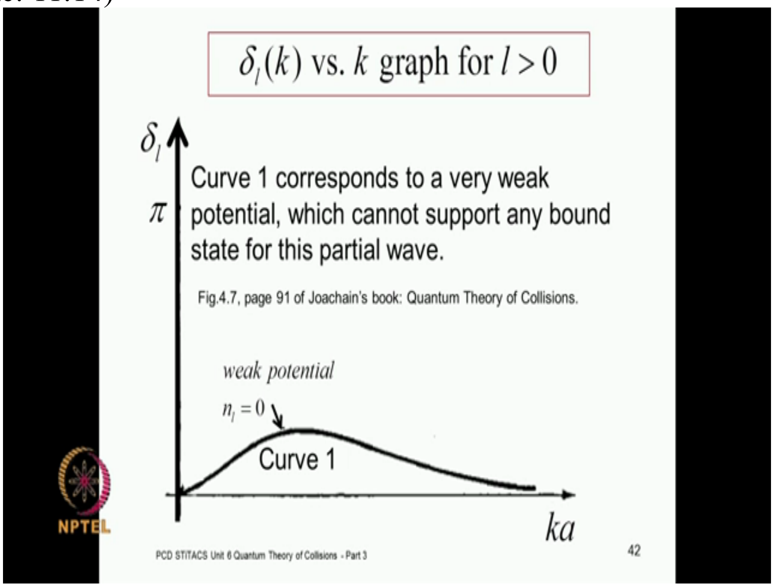

Is the fact that in the case of l = 0, for the s waves, what happens is you get virtual bound states, okay, you remember, that, that you had virtual bound states for l = 0 when you have the resonance condition at, where the depth and the scattering strength parameter was pi by 2, you got virtual bound states.

Whereas in this case for higher orbital quantum numbers, you get proper bound states, so it is not it is not like a state which is half bound and half not bound which was the case for the l = 0 case. So, now, if you have a weak potential the phase shift will first increase, if it is weak.

It, if the potential is so weak that it cannot even hold a single bound state then the phase shift will first increase.

And then, since there is no bound state at all, it will have to come back. And eventually go to zero. But then, as you increase the depth of the potential or the range of the potential make the potential stronger. We have seen these plots for l = 0. So, now we are observing that for l equal to, greater than zero. We have somewhat similar plots. But then, we have some differences also.

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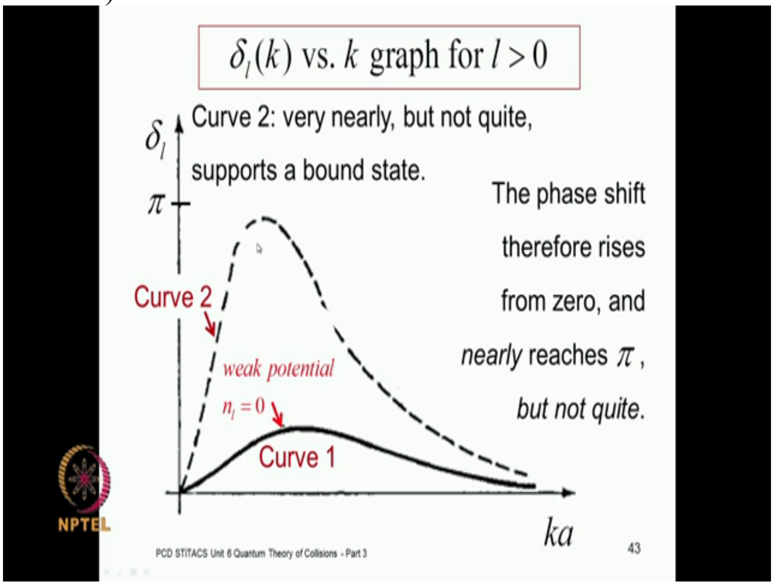

Because as the potential becomes stronger then the phase shift increases. But does not quite get to pi, unless, it actually is strong enough to hold a bound state. Then it flips over and then comes back whereas if the potential becomes stronger still.

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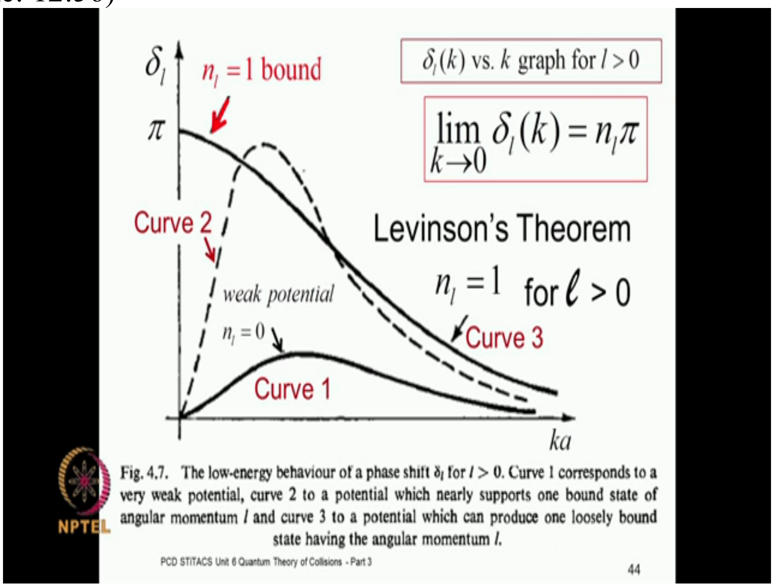

Then, the once it crosses that threshold. Then, you have a one bound state. So, that the low energy phase shift will become equal to n pi, n = 1, in this case so that it is just strong enough to hold one bound state. So, the phase shift at low energy limit, the phase shift will be equal to pi and then it drops which is given in the curve 3. So this is completely along in consistent with the Levinson theorem,

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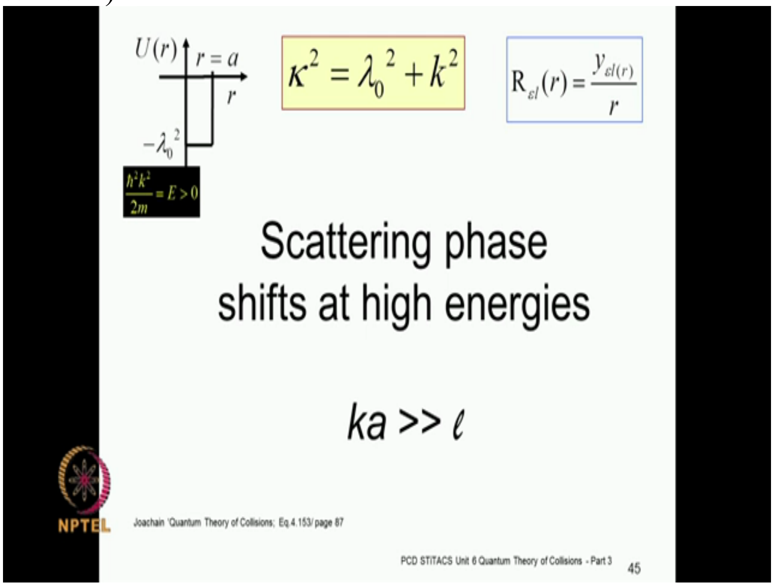

What we will now consider. We consider the low energy behaviour. Now, we will consider the high-energy behaviour okay. So, high energy, high wave with respect to what? High with respect to the orbital angular momentum, because ka and l, they come together. So, any comparison between them tell, tells us that ok if you are much above the l value. Then you are in the high energy domain so far as this context is concerned.

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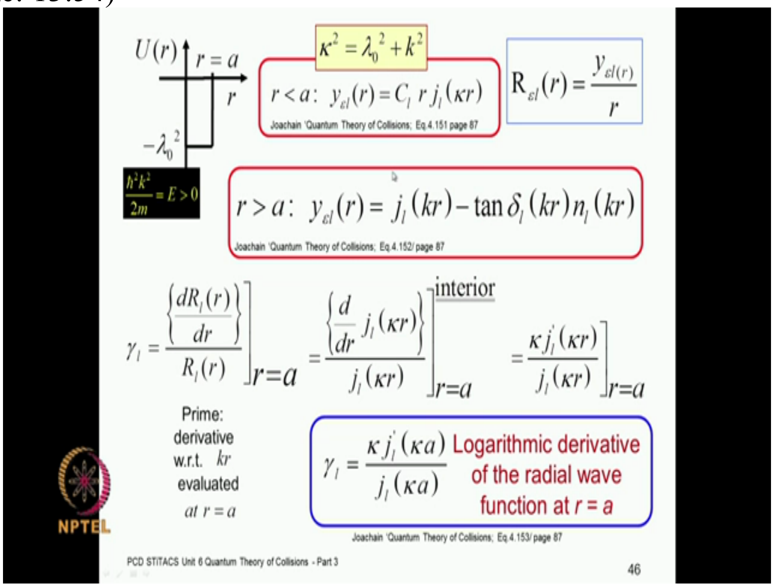

So, in this case, let us set up the relationships for the Schrodinger equation, for the inner region you are said the, the actual radial solution is capital R. You set up the differential equation for y, the radial solution being y over R. So, you have got these two solutions for the inner region and for the outer region, the outer solution will be determined by the scattering phase shift, okay.

And you have got from the continuity of the wave function. And it is derivative at the boundary, this continuity of the logarithmic derivative okay. And this must be the same for the inner region as for the outer region. So, you have kappa square is lambda 0 square + k square.

So, this is the same kind of parameter that we have considered earlier. So, what do we get? The logarithmic derivative must be continuous and at r = a it must be kappa. It will be given by this kappa a.

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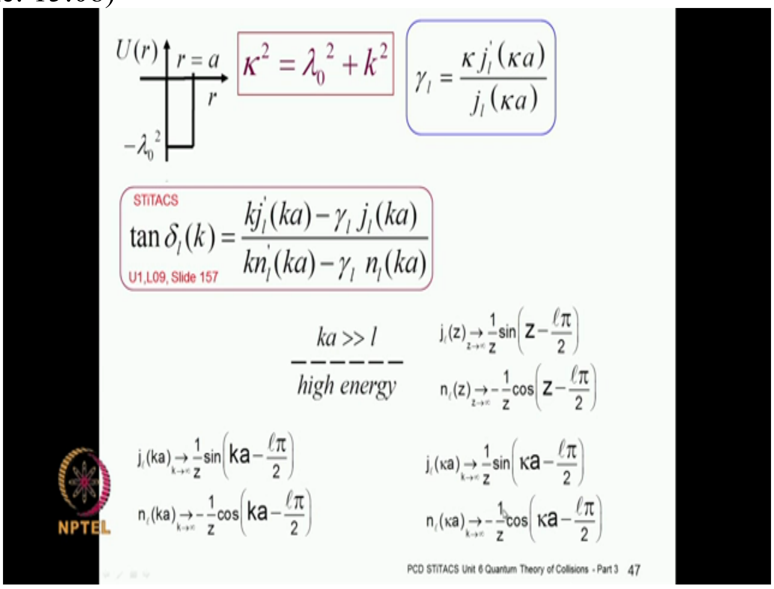

So, let us take this. Now, I will use these relations which we have obtained earlier. This was in unit 1. So, we have obtained this relation earlier. So, I will use that relation directly and consider the high energy limit. So, the high-energy limiting Bessel function values are given by a sine of z - l pi by 2 divided by for the Bessel function.

And the Neumann function is a cosine function with the same argument with a 1 over z again, but with a minus sign okay. So, these are the usual relations for the Bessel functions and Neumann functions which we have to substitute in this relation. So, let us substitute these values.

So, now you have to put in the value corresponding to ka whereas for gamma, you have to substitute the value corresponding to Kappa a. So, you have these values here, ok. So, there are similar relations but then, this one is k and this one is Kappa.

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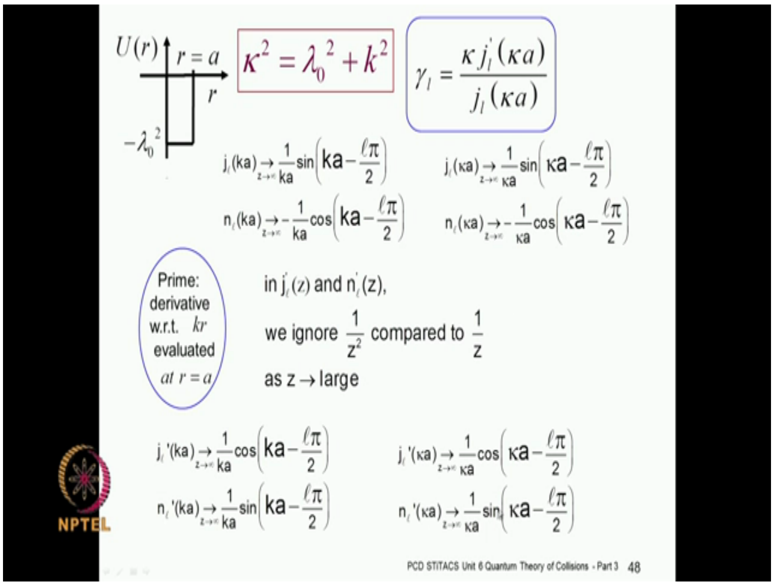

And with the k's and the Kappa's taken care of what have we ignored? We have ignored for large z, terms of the order 1 over z square, when they come together as additive terms with 1 over z terms. So, that is the approximation. But that is fine mean that always approximation we take for the asymptotic limit.

So, so, here the asymptotic limit is coming because, not because of the distance, but because of the energy parameter, that this is the large energy limit. So, you have a similar consequence on the values of the Bessel functions. So, you put in these values okay and get the expression for gamma.

So, these are straightforward substitutions I will not comment on this. And now here, this angle kappa a -l pi by 2 is what I write as Phi, just to make our notation compact, ok. So, I will write this expression in terms of the cosine, sine and tangent or cotangent of the angle Phi as it the case would be.

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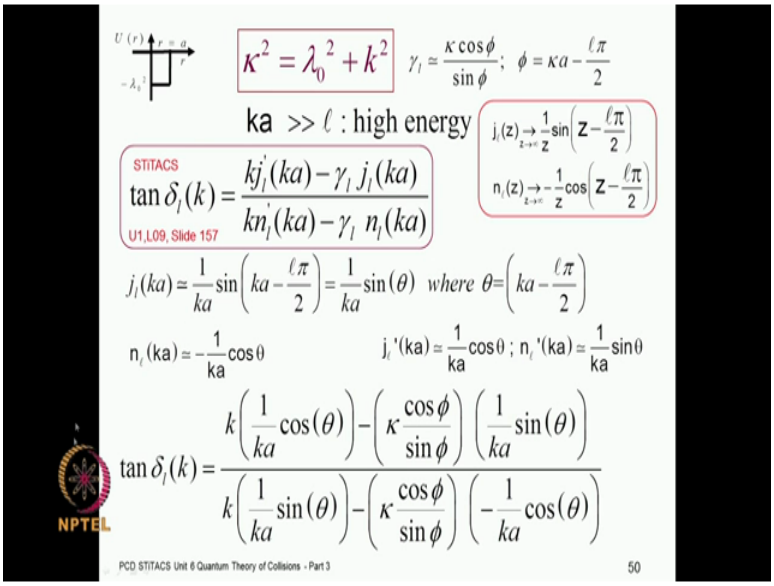

So, I introduce the symbol Phi just to make our notation a little compact. So, this is gamma here in terms of Phi, which is this angle kappa a - l pi by 2. Or in terms of this, we can write our earlier result. So, now the tangent of the phase shift is now given in terms of the trigonometric functions of theta. Theta is ka - l pi by 2 and the other angle is Phi which is Kappa a -l pi by 2. So, these are the two angles which come in our expressions the actual substitutions are straightforward.

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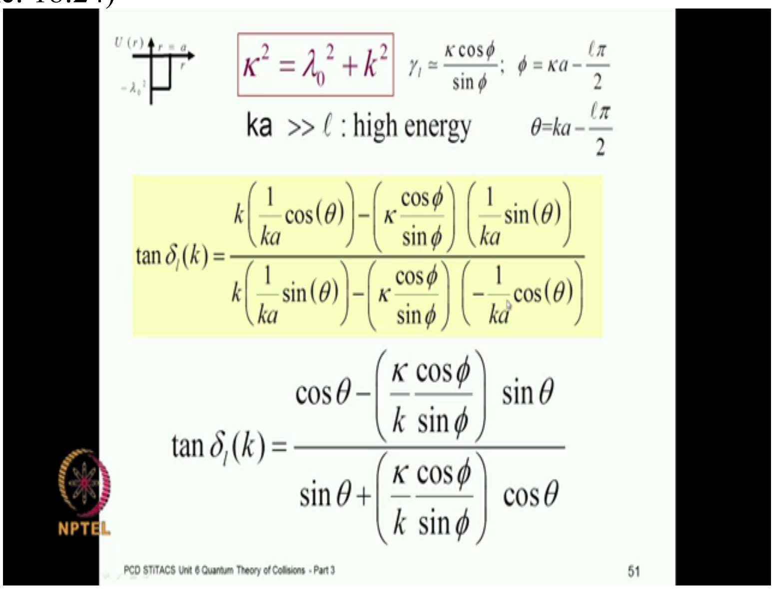

So, we have written them in terms of theta and Phi and a little bit of substitution as you can see this cancels this k. The 1 over a is in every term, in the numerator as well as the denominator. So, they are going to cancel, right. So, now you get rid of all the 1 over a.

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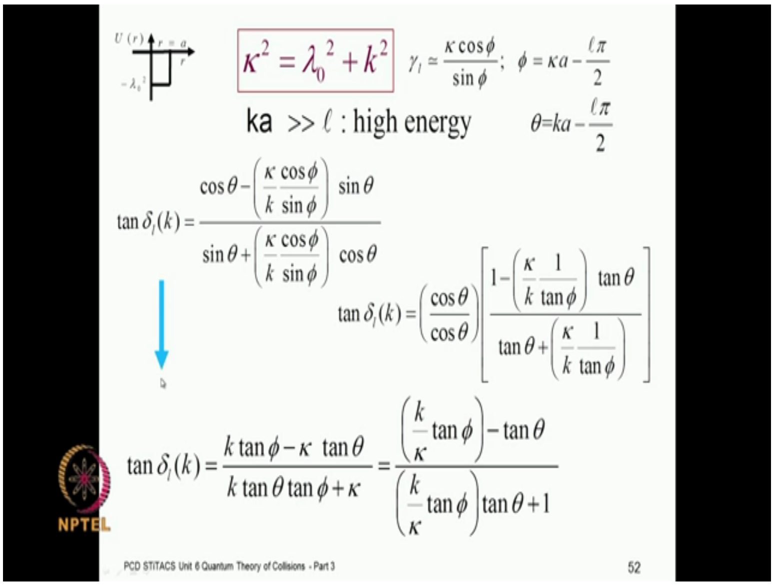

And you get after these simple substitutions. A little bit of rearrangement as you can now recognized by this blue arrow that there is nothing more in it than straight forward substitutions. So, I will not take you through this step-by-step. But you can work it out and you can always refer to the PDF for details.

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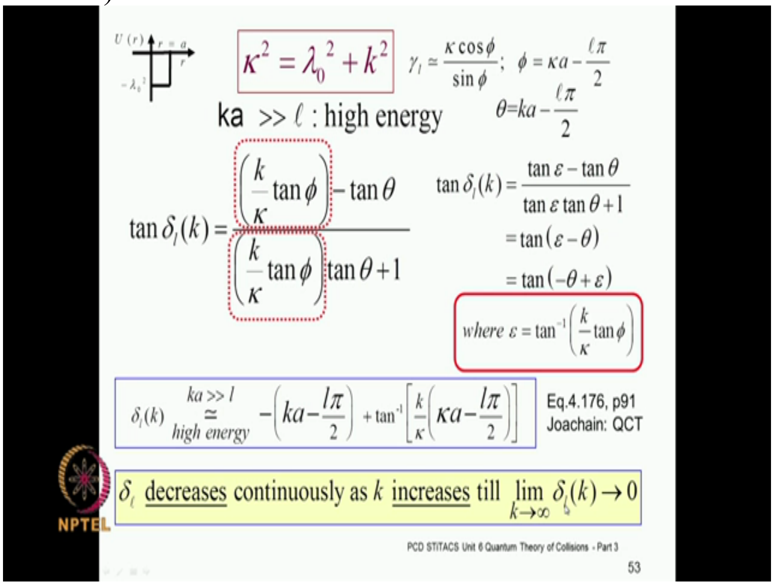

So, here you are. So, this is the expression for the tangent of the phase shift and it appears in terms of two angles theta which is k - l pi by 2 and Phi which is Kappa a - l pi by 2. Now I see that there is a k over kappa times tan Phi. So, I introduce this angle epsilon the tangent of which is k over kappa tan Phi because that will make it possible to write the tangent of the phase shift in this form.

So, that you can write it as the tangent of a difference of two angles, okay, so that is the idea. So, we introduce this epsilon so that you can write the phase shift or the tangent of the phase shift as tangent of another angle. And, and you can immediately get the two angles; you can equate the two angles. And you get the high energy limit which is - ka - l pi by 2. Now, this is the one of the two angles this is the theta and then you have got the Phi over here.

But now the Phi in terms of Phi you have the epsilon so you get this k over kappa, kappa a - l pi by 2, right. So, this is the expression you get for the phase shift at high energy. So, as energy increases, you have this -ka, right. So, the phase shift will keep continuously decreasing till it becomes 0, okay. So that is the high energy behaviour.

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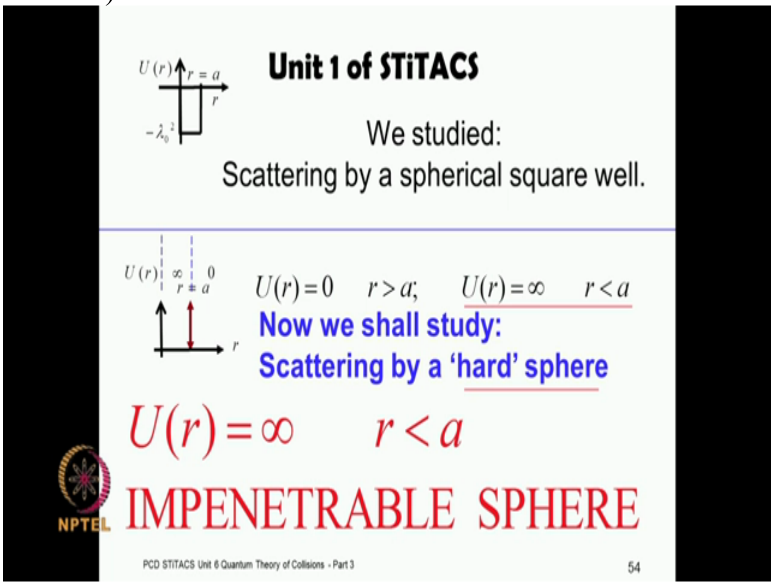

Now, we will now take the example of a square well, we have already considered but we have considered square well potential with finite depth and so on. So, we will now consider a rigid potential like an impenetrable sphere okay. It is a, it is sometimes called as a hard sphere.

You cannot penetrate it because the potential inside in the inner region from zero to a is infinite. So, nothing can get it, okay. It is, it is an ideal situation; it's a mathematical construct that the potential is infinite are no scattering, no projectile can penetrate that. So, we will consider this case of hard sphere scattering.

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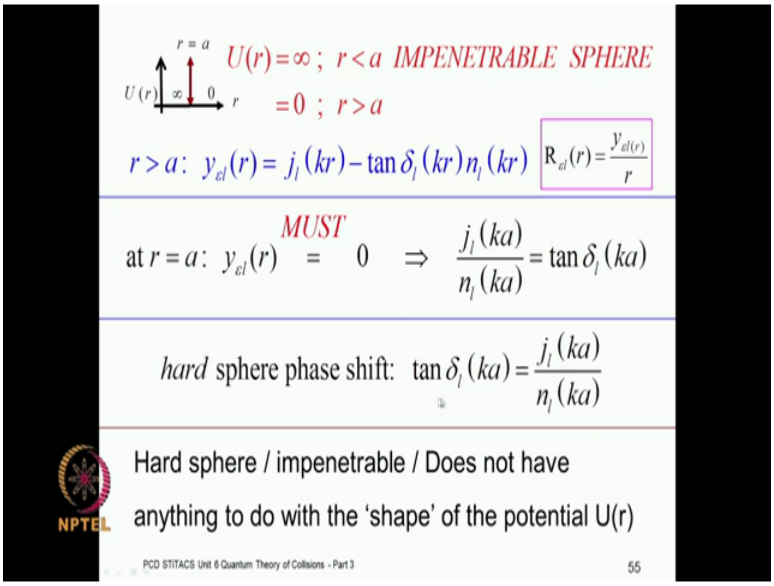

Now, in the case of the hard sphere scattering, we are not bothered about anything like the shape of the potential or anything because it just does not matter; it is infinite. So for this inside there will be it will be impossible for the projectile to get in and outside it will be governed by this phase shift.

What happens at the boundary? It go to zero because it cannot get in, okay. So that is a boundary condition because it is hard sphere; it is impenetrable. And therefore at the boundary r = a it must vanish. And therefore this j l k a over n l k a must give you the tangent of the phase shift. So, now we have an expression for the hard sphere phase shift.

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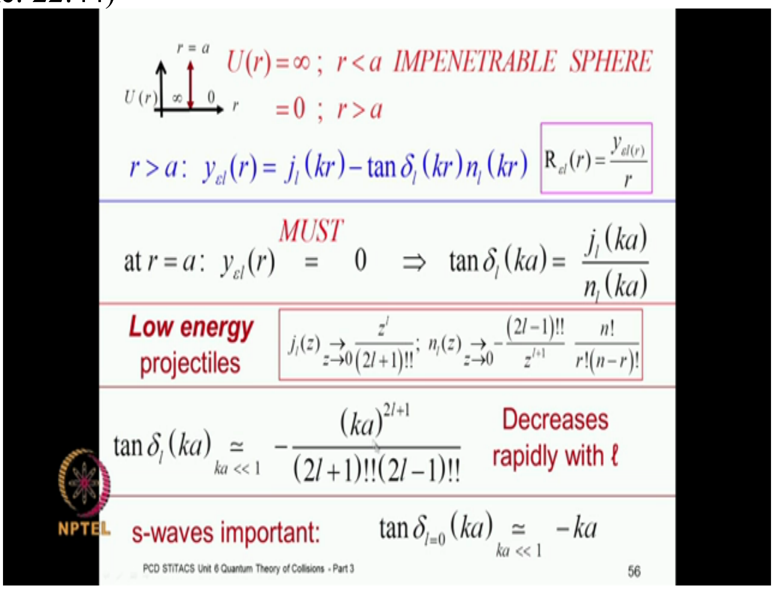

Now, this is an important result because when we deal with any arbitrary potential, we can pretend as if this potential is made up of two pieces. One of which is a hard sphere kind of situation and the other contains the dynamics. So, we will break up the net result into this kind of analysis. But that is something that we will discuss in subsequent classes.

So, for now, we know that the function y must go to 0, at r = a, which gives us this expression for the tangent of the phase shift. And now, over here, if you now consider the low energy limit then, in the low energy limit, you know, that the Bessel function what the limiting behaviour of the Bessel function and the normal functions are, for the low energy limits as it tends to 0.

You can put them in and again you get the same ka to the power 2l + 1 behaviour from this, right. So this is the low energy limit for a hard sphere scattering. And you can see that it decreases quite rapidly with l again in consistency. No, it is completely consistent with our expectation that higher partial well waves will not matter.

Most of the scattering will be determined just by the l equal to 0 the s phase. So, this one, this is your result which you will remember for l equal to 0. We have found that it goes as - ka because l for l = 0. This 2l goes to 0 and then you will simply have the tangent of delta 0 going as -ka.

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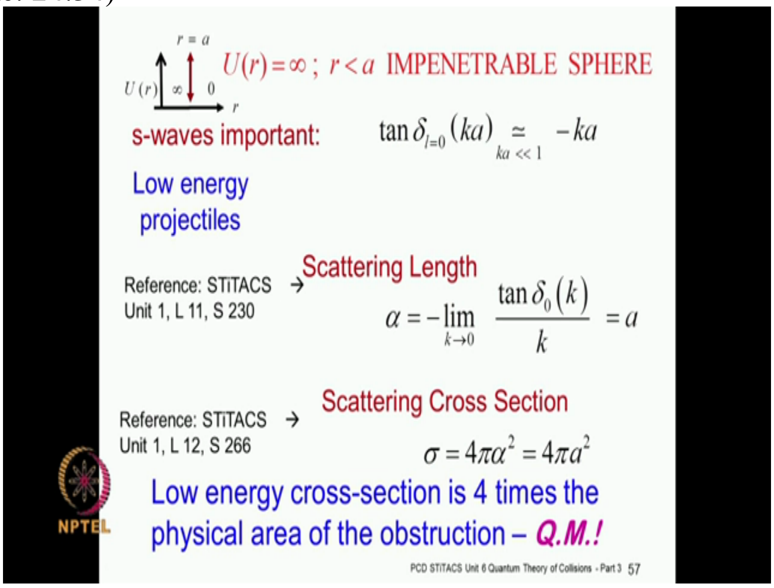

Now, notice that in this case the scattering length which is the ratio of tan delta by k, it will go as a; and if the scattering length is alpha what does it give us for the scattering cross section? It is four times pi is a square the classical cross section is pi times a square, okay. Pi a square that is the area of a circular disc of radius a.

So, this is four times that and that is, that is not surprising because this is not classical this is quantum so obviously you will expect some differences. And this is what it is.

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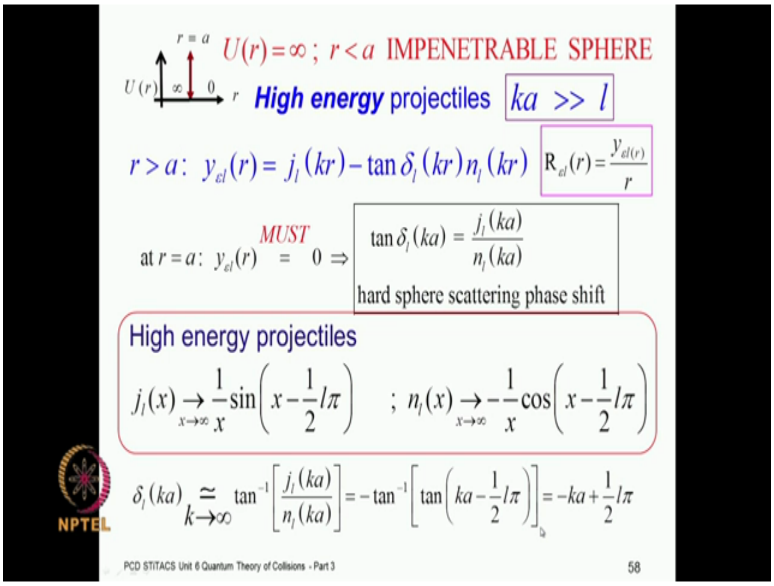

So, now you consider the High energy projectiles. Now, when you consider the High energy projectiles, we have seen that at r = a, this function must go to 0 that this is the hard sphere scattering phase shift. And the high energy projectiles again you use the High energy limit for the Bessel function and the Neumann functions.

So, you can put these expressions over here for the tangent of this angle. And what does it give you for the phase shift itself is this tan inverse of this ratio. This ratio itself is tangent of this. So, you get the phase shift to be - ka + half l pi.

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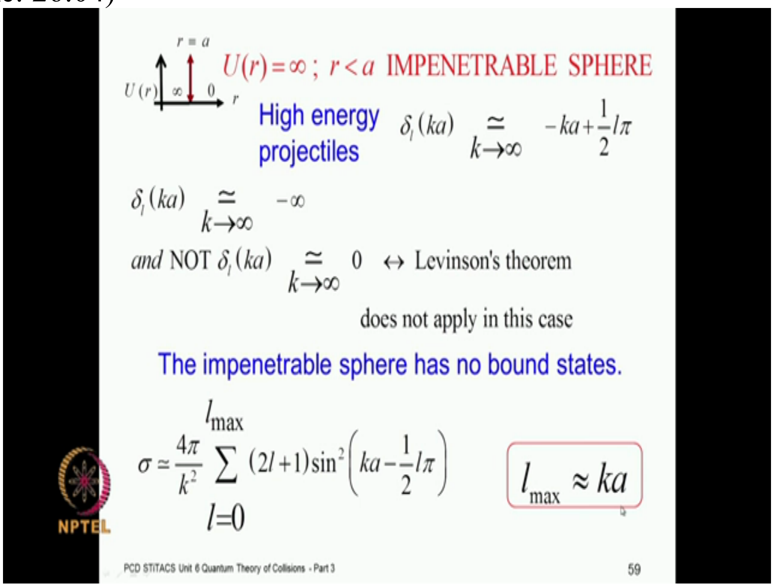

Now, this is an interesting result because what is happening is that in the Levinson's theorem, we always argued that the phase shift at high energy would go to 0, right. That was the reference for the angle that we considered whereas in this case, the phase shift keeps becoming more and more negative. And it goes to negative infinity okay.

So, this is something which you might think is not consistent with the Levinson's theorem. But why does it even have to be consistent with the Levinson's Theorem, because this is a hard sphere. It does not have any bound state, okay. So, there is, the, there is no problem with that issue over here.

So, this has got no bound state at all. And again you can get the total cross section by carrying out the summation up to the maximum value of l which using our semi classical argument, we know, is of the order of ka. So, for all practical purposes, we can take l max to be equal to ka. It works in most situations which I have mentioned earlier in various different contexts.
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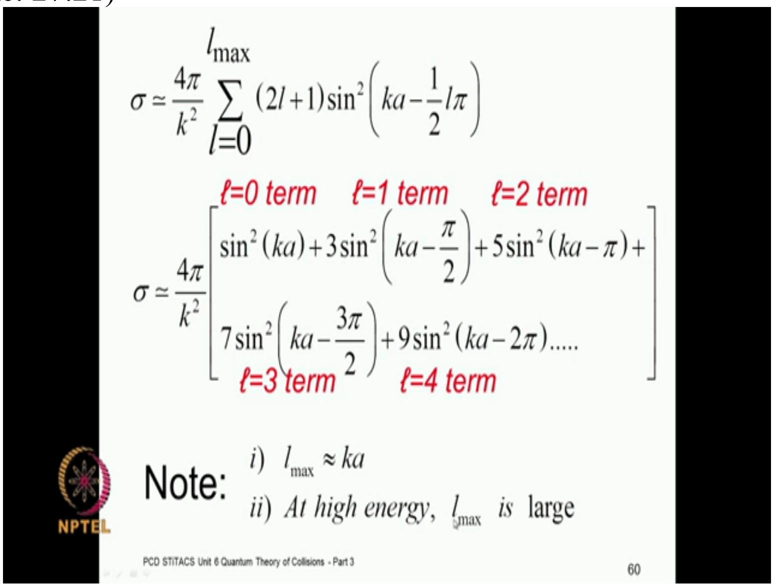

So, this is the cross section that you get partial wave contributions from different values of l. You do not have to sum all the way to infinity. You just have to go as far as l max which is above ka. And what does this some turn out to be. So, let us take this, term by term. So, let us write this expansion explicitly, because you will find that it sums up to a very compact result which is rather attractive. So, it is nice to get it in that form.

So, you write all the terms for l = 0. This half l pi is the only thing which is going to be different in every term, okay. You are summing over l going from 0 to l max and this half l pi will go from 0 to pi by 2 and so on, right. So, you get for l = 0, a term in sine square ka. Then, for l = 1, you have got three times, you have got a 2l + 1 factor here; so, three times sine square ka - pi by 2.

Then, for l = 2 you have got to l + 1, which is 5 times sine square ka, - pi, okay; for l =2. And that is how you get various terms. So, you get with different coefficients of the sine square functions 1 over here, 3 over here, 5 over here, 7 over year, 9 over here. Notice the, the pattern in which the coefficients are coming so that you can generalize it very easily.

You can go to higher order terms. So, the maximum value that you have to consider is of the order of ka and at high energies l max can be large. So, you can sum up to all those values.
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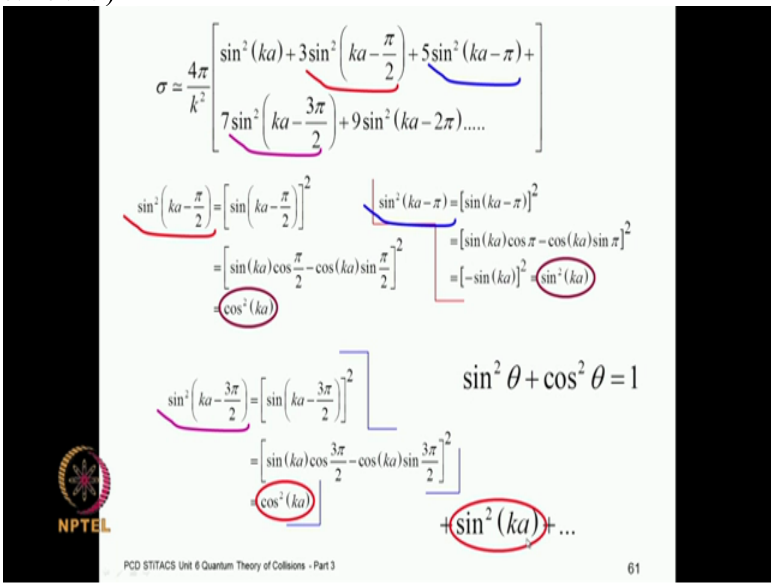

So, this is the pattern that you are getting and this angle which is sine square, this is not just theta; but it is theta - pi by 2. So, the argument is ka - pi by 2. But you can write it in terms of sine or cosine of ka itself; because sine square of ka - pi by 2 is nothing but the cosine square of ka. So, you can simplify this.

Likewise, this is sine square of ka - pi and this simplifies to sine square of ka, okay. So, all of these angles can be written very simply, in terms of sine square or cosine square of ka. So, this comes out to be sine square ka, the sine square ka - 3 pi by 2, which is here. So, this term comes out to be cos square ka.

And then, you get terms in cos square ka and cos sine square ka together. So, you can combine them and accept that sine square theta + cos square theta = 1 even in atomic physics, right. So, we can simplify this relation and we really get a very simple sum. But, of course, we have to take care of the coefficients here, because they are not the same.

You have got 1 over here, 3 here, 5 here, ok. So, keep track of that and we will make use of this relation. So, let us look at these terms. So, the next one again I have not written all the details over here. But then, you will get similar combinations and you will get either sine square theta or cos square theta where theta is ka.
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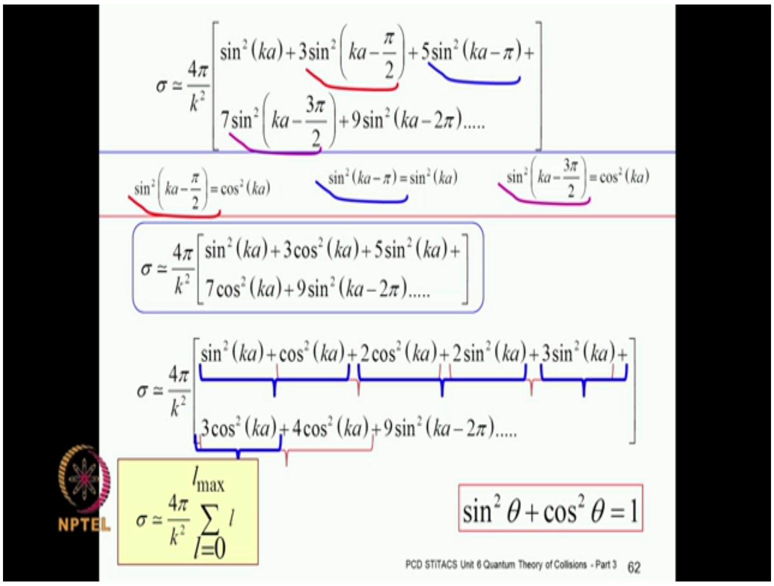

So, these are the terms that you get. So, this one is cos square ka. Here you have got sine square ka. And here you have got cos square ka and so on. So, now, you write these terms in terms of this angle ka now. No matter what value of l is, okay. It is always written in terms of sine square or cosine square of ka.

And now, you have this factor 3. This is 3 times cos square ka. So, this 3, I split into 1 and 2. So it is cos square ka + twice cos square ka, so that I can combine this cos square ka, with this sine square ka, to get unity. And then I can combine this twice cos square ka, with the twice sine square ka, which I am getting from the next term to get a sum, a factor of two, okay.

Because here, I have got 5 sine square k a, which I have split into twice sine squared ka + 3 times sine square ka, so I take this to twice n square ka, with this twice sine square ka and this 3 sine squared ka, with this 3 cos square ka of the following term. So, this is just a rearrangement of terms so that I can combine these to, to get a simple result. And what you see is that we are simply adding 1, +2, +3, +4, +5 and so on, right? up to l max, right.

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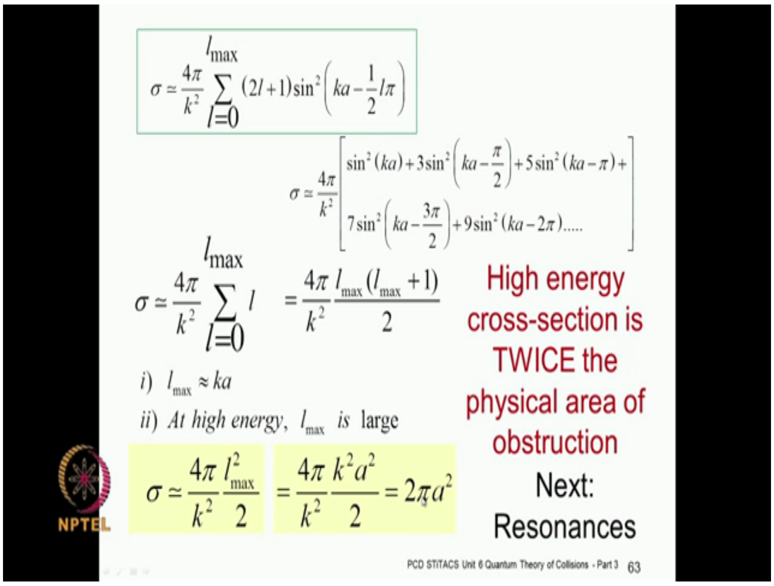

And that sum, you can easily get to, l max into l max + 1 by 2, okay. So, that is the compact expression for the scattering cross section and you find that it is determined only by this upper limit in this particular case, okay. So, this is the case, that we have considered and when l is large. Then, you can approximate this to be l square by 2, okay.

If you ignore this one compared l max, because l max is large, it can be 10, it can be 20. So, you get the high energy cross-section. And in this case, now, if you put this equal to l square over 2, what do you get? Twice pi a square. So, this is half the previous result. This is twice pi a square. The previous result was 4 times pi a square.

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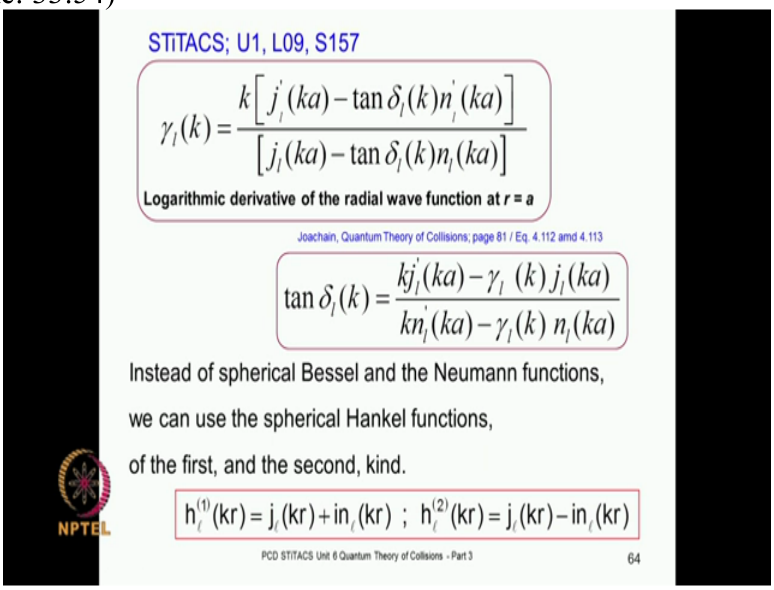

And now, we can consider the resonances. So, once again we go back to this expression. So, this is a common expression that we are going to use throughout our analysis. That is the basic relationship to discuss the phase shifts. But what we will do is, we can use any pair of base functions. Our base pair has been the Bessel function and the Neumann function. We can also use the Hankel functions.

The Hankel functions of the first kind and the Hankel functions of the second kind, because they are made up of the Bessel and the Neumann functions. And you get an alternate pair of basis so that it gives some advantage. So, you have got the Hankel functions of the first kind which is just the Bessel function j + i times.

And so you have got the Bessel function + i times the Neumann function, in the Hankel function of the first kind; in the Hankel function of the second kind, it is the Bessel function - i times the Neumann function, okay.

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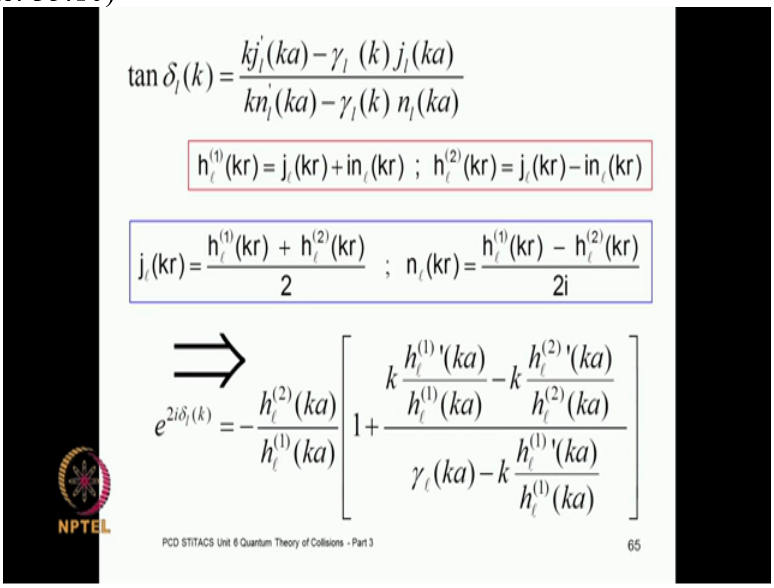

So, in terms of the Hankel functions, now, we can rewrite the expression for the tangent of the phase shifts because the Bessel functions and the anointment functions can be written in terms of the Hankel functions backward, right. So, you substitute all that and then you get the phase shifts, okay.

And you get an expression for the phase shift which is now given completely in terms of the Hankel functions, okay. So, this is again straight forward substitution which I will let your work out. This is the result that you get, that the scattering phase shift is given by this expression here.

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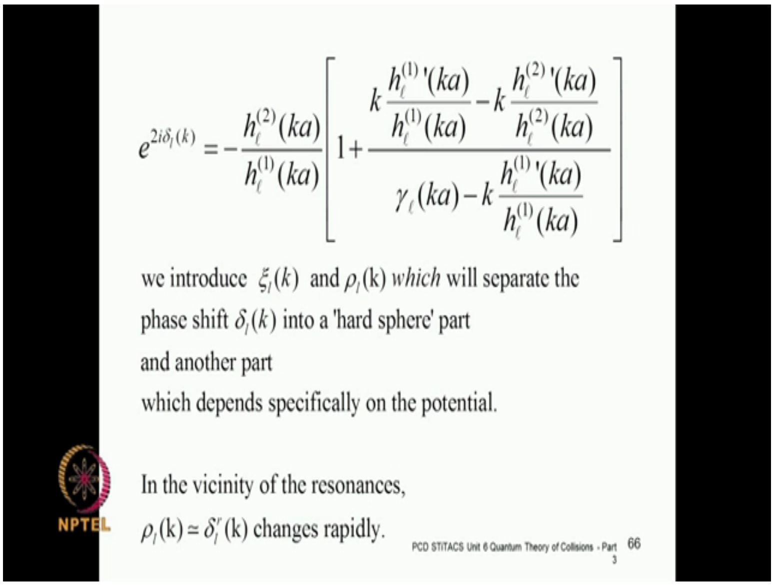

Now, the reason to put it in this form is, will, become clear perhaps in the next class or maybe in the next one or two classes. Because what it allows us to do is, to introduce two different angles. And you can write the phase shift, the, the net scattering phase shift is delta. But you can write this scattering phase shift in terms of two angles, okay.

You can write the scattering phase shift as a sum of two different angles. One is Xi and the other is Rho. So, we introduce these two angles. And one is defined in terms of the ratio of the Hankel function of the second type, to the Hankel function of the first type which you see is factored out in this term already, right.

And then, you have got the other factor, in terms of which, we will write another angle which is Rho, so that the scattering phase shift can be written in these two parts. And then, it turns out that these two parts refer to hard sphere scattering and the other will be given by the actual dynamics of the potential.

And that is the one which we be, which will be of central interest in considering resonances; because when you have a resonance, the other term which is Rho, which gets added to Xi, is the one which will very rapidly at the resonance. And it is this rapid variation in the resonance region which is going to be the subject of a discussion in the next several classes.
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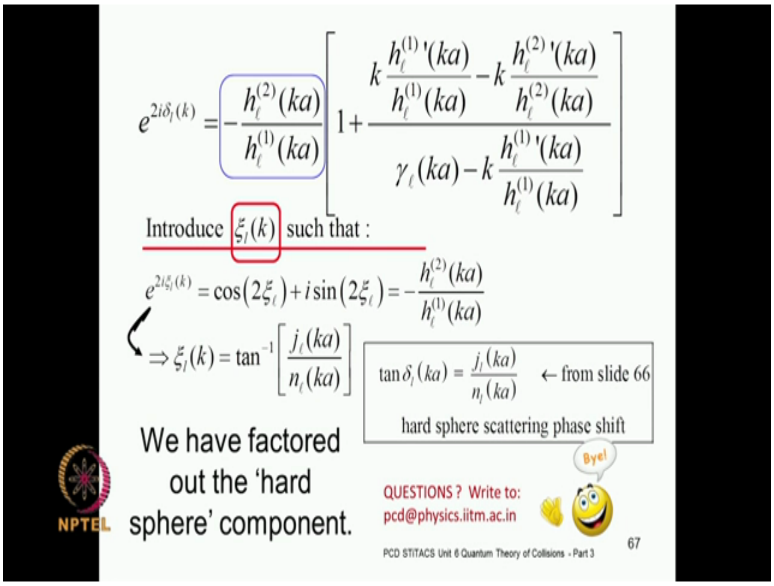

So, this is the phase shift in terms of the Hankel functions, we have introduced these two angles. Now, one is Xi. And this Xi is written in terms of, this ratio of the Hankel function of the second type, to the Hankel function of the first type, together with a minus sign. So this e to the 2i is Xi l is now, defined. This is the defining relation, for this particular phase shift, okay.

This is a part of the phase shift. So, this is one part of the phase shift. And then there is the other part, You will see immediately that the hard sphere scattering phase shift which we obtained earlier was nothing but this. It was exactly this. So, we have factored out from the total phase shift one part which is coming, which can be attributed completely to the hard sphere component, okay.

So, it is not that there is a physical hard sphere which is sitting over there, okay. What this analysis is letting us do is, that the net scattering phase shift which is determined by the real potential, by the real dynamics of that potential. So that real potential generates a result, a resulting scattering phase shift which you can write as a sum of two terms: one of which can be attributed to hard sphere scattering.

Because the ratio that you get which in terms of which you define the phase shifts Xi gives you for its tangent, nothing but the same ratio that you get for scattering by a impenetrable sphere, okay. This is just the ratio of the Bessel function to the Neumann function okay. So, this result we have from an, from the earlier discussion.
That this is the hard sphere scattering phase shift and now what we will do in subsequent classes is to focus our attention from the hard sphere part to the other part which is the Rho,

okay. So, there are 2, 2 contributions to the net scattering phase shift: One is what we will call as the hard sphere component and the other is the dynamical component.

And the dynamical component in the absence of resonances will very smoothly with energy or it will have a smooth variation with respect to k. But at resonance, it will change very rapidly. So, these are the resonances which are of great importance for our study in collision phenomena.

There are two kinds of resonances. You have got the shape resonances and you have the Fano Feshbach resonances. So, these we shall discuss in the next few classes. So, there is any question I will be happy to take otherwise we take it from here in the next class.