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

Prof. P.C. Deshmukh
Department of Physics
Indian Institute of Technology-Madras

Lecture 09
More on: Phase shift analysis

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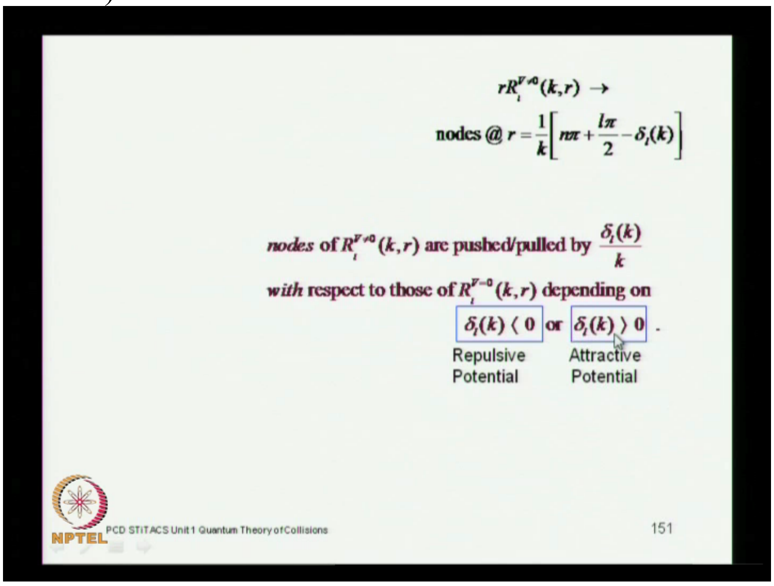

Greetings, so we had some discussion on the phase shifts and what kind of information they bring to us when you perform a collision experiment. And in particular we saw that when you have a phase shift and what it does is here, so this phase shift will change the position of the nodes of the radial function this is what we discussed last time.

That nodes of the radial wave function are either pushed or pulled depending on whether the potential is repulsive or attractive. With reference to which the phase shift is either negative or positive. So, when the phase shift is negative in the case of repulsive potential then the nodes are pushed away otherwise they are pulled inward, inward is toward the center of the scattering potential.

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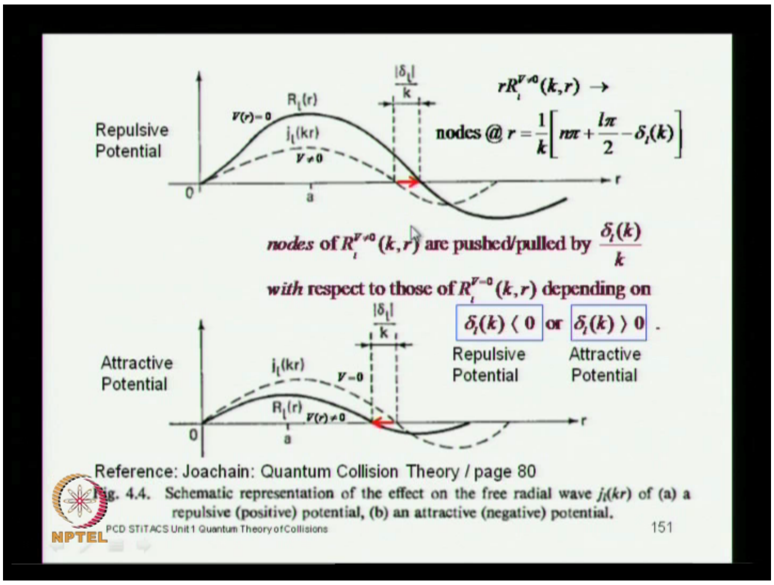

And this is the general picture that emerges and we clearly see that the phase shifts carry valuable information about the target potential itself.

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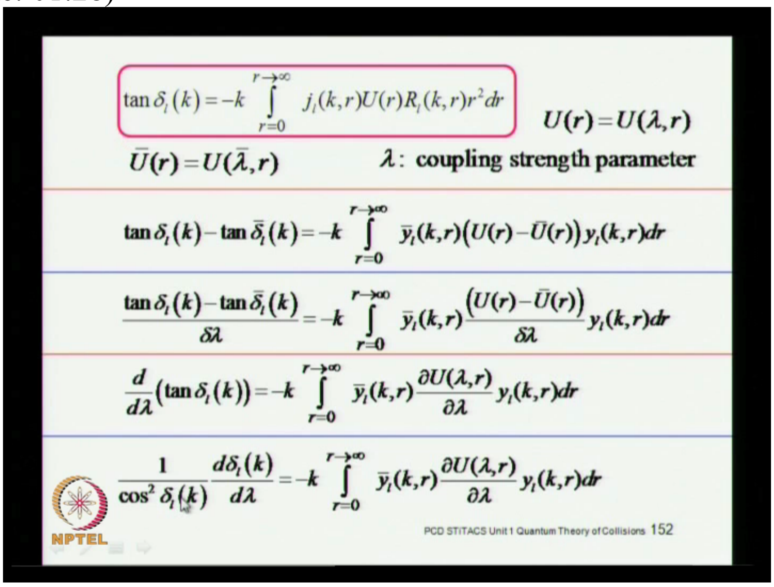

Now what we will do is to analyze the formulation a little further and the phase shifts we know is an angle. And typically angles are known modulo pi. So, if you either subtract pi in mathematics usually you are not able to see the difference. Because you know there is just a sign inversion of various terms which come in and it is not modulo pi.

So, you can add 2pi, 3pi, 4pi, 5pi and so on. And you really do not get any exact idea about what the actual phase shift is. An absolute value is something that you would like to define and there is a way of doing it by introducing a mathematical construct. So, let us introduce a coupling parameter like lambda okay.

Now this is not a physical switch it is not like a rheostat or some regulator that you have to control the strength of the interaction. Because the strength of the interaction is determined by nature itself but this is a mathematical construct and you define the potential such that you introduce a parameter lambda on which you have got a mathematical control.

And you can now talk about two different potentials. One with a value lambda and another with a value lambda bar at this potential we will indicate by a U bar, so a bar on top of it is the potential this is the reduced potential mind you. So, this is the reduced potential corresponding to the control parameter lambda equal to lambda bar. Now this relation is valid for the tangent of the phase shift we derived this in the previous class.

We will use this now and we will now have a similar expression not just for the potential U but a similar expression for the potential U bar for exactly the same reason. So, you will have identical relations for U and U bar and if you take the difference you get the difference between these two tangents okay. And the difference in the phase shifts delta and delta bar or rather difference in their tangents.

Is then given by this integral in which you have got the functions U and U bar okay. So what you can do now is to divide this difference by delta lambda which is your control parameter and then you can take the limit delta lambda going to zero. So, you will get the rate at which the phase shifts or rather the tangent of the phase shift changes with your control parameter. So, now we take the limit delta Lambda going to 0.

And that gives you the derivative of the tangent of the phase shift and this is the only parameter U is the only thing which depends on lambda. So, you get the rate at which the potential will be changing with respect to lambda in the integral, so this appears in the integral. Now you take the derivative of the tangent function and you get the derivative of the phase shift itself with lambda with the 1 over cos square term.

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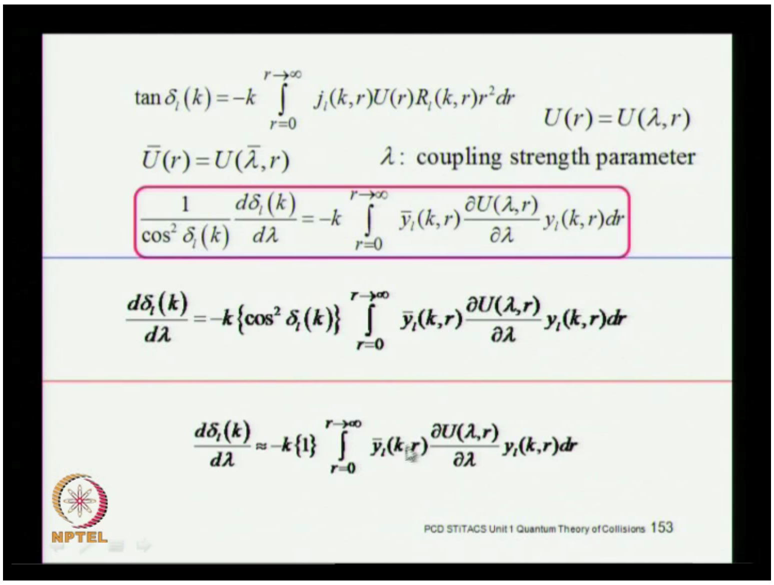

And cos square delta for small angles it will be nearly equal to 1. If the phase shift is very small, so if you move this cos, cos square function over here, you can approximate this bracket nearly equal to 1. So, you get a relation which is approximately correct very nearly so for small phase shifts. That the derivative of delta with respect to lambda is given by this - k times this is a factor of 1 and then you have got this integral right.

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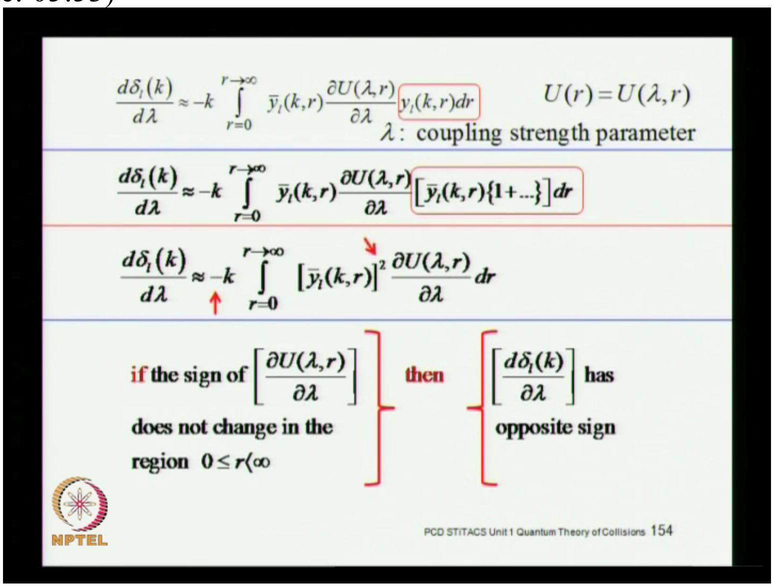

Now notice that lambda is just a mathematical strength parameter. But when you do the calculations you can assign a certain value to it okay, when you simulate this in a quantum mechanical model. And then you can introduce a coupling parameter and this function which is the function corresponding to the potential to the unbarred potential this is the wave function corresponding to the U bar potential right.

And this function you can expand around y bar okay. Because the wave function when you have a certain potential because what you can do is let U bar go to 0 which is no potential at all which is the free particle okay. So, if you get, let one of these go to zero then the other potential will tell you how the phase shift responds to that potential.

So, this wave function it will not be very different from y bar and you can take the leading term and what this gives you is the square of y bar okay. And you can always choose y bar to be the same as the spherical Bessel function or the solution for the free particle. So now let us see, let us examine this relation, here you have got a square in the integral okay.

The integrand consists of this it is a product of two factors one of which is a square which is always non-negative it is always positive right. The other is the rate of change of the potential with lambda. And then notice that there is a minus sign over here, now what this means is that the value of this derivative if this sign is not changing in this entire range 0 through infinity.

Then the sign of this d delta by d lambda is opposite to that of the sign of del U by del lambda. The reason it is opposite is because there is a minus sign here the other factor is positive and this, its value it does depend on r. But we are presuming that this derivative of U with respect to lambda is not changing its sign in the entire range of integration okay. So, d delta by d lambda will have opposite sign.

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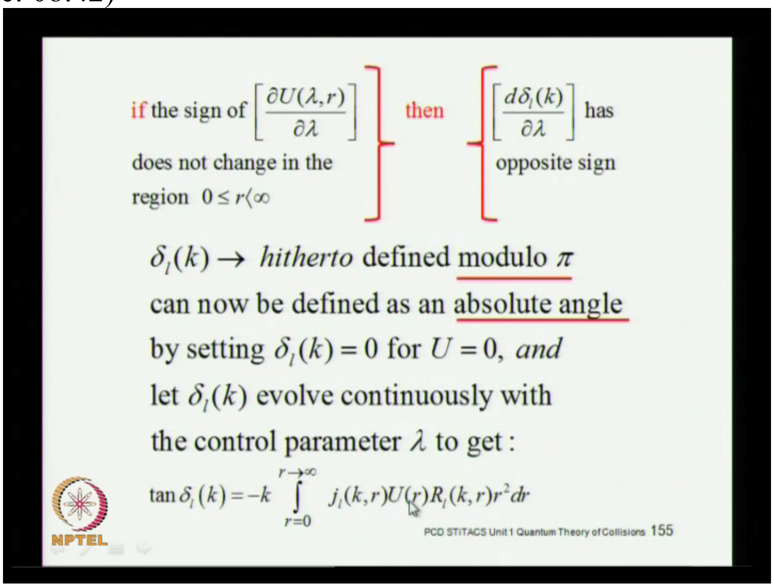

Now what this helps us is the following that this phase shift which is defined modulo pi can now be defined in an absolute manner. Because we can take we can set the value of delta that angle to be equal to zero when U =0 okay. So, this is like calibration in a certain size that is fixing the zero of the phase shift.

And once you fix the zero of the phase shift then let that phase shift evolve the way it would and it will change from zero. So, it will the ambiguity of modulo pi phase shift can be removed by this mathematical trick using this control parameter. So, this is the tangent of the phase shift and this is the expression that we get for the potential U. And this is the expression which we can really use to carry out our phase shift analysis.

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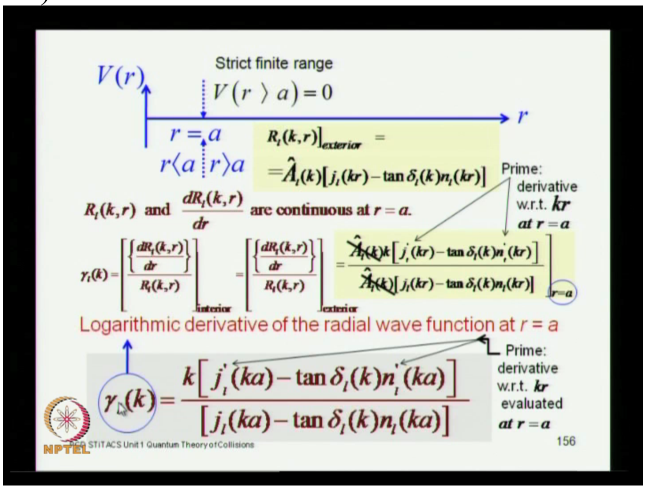

So, now let us consider a potential which has got a strict finite range which means that beyond this range r = a. The potential is zero this is what is meant by a potential having a strict finite range and many scattering potentials are of a similar nature. Some of them do not have a straight finite range but they have a range which is not so strict.

But nevertheless you can find a region of space beyond which they have practically no influence because any physical potential does have; you know diminishing influence the farther you go away from it. So, in this case the exterior solution which is the asymptotic solution this is the solution as r tends to infinity right. Now that is going to be the nature of the solution in the exterior region.

And that we already know from the outgoing wave boundary condition is given by a superposition of the spherical Bessel function and the Neumann function. And it is mixed in this proportion which is determined by the potential via the phase shift it generates rather the tangent of the phase shift it generates right.

So, this is the radial function in the exterior region and what we know is that the function and its derivative must be continuous in the entire space right. The Schrodinger equation is a second order differential equation, so the wave function and its first order derivative is continuous in the entire space.

So, there must be continuous at r = a as well. So, inside this region in the small r region, even if we do not know what the potential is, even if we do not know the exact nature of the wave function. We do know that whatever be the wave function the wave function and its derivative must be continuous at r = a right. So, this we can say this in terms of the logarithmic derivative of the radial wave function at r = a.

That this logarithmic derivative must be continuous at r = a and if you evaluate this derivative in the interior region it must be the same. In the exterior region we do not have much information about the nature of the solution nature of the radial function in the interior region but we do know what it is in the asymptotic region in the exterior region.

So, we can use this exterior wave function to get the logarithmic derivative by taking this dr by dr divided by the radial wave function in the exterior region and evaluate this at r = a. So, let us do that and the derivative of the radial function in the exterior region is the derivative of this. So, this is j prime, prime denotes derivative of the Bessel function with respect to its argument okay.

And since the argument is kr the derivative then gets multiplied by a factor of k okay. So, that is how this k comes so that is the notation we are using. So, you get, this is some energy dependent normalization a carrot or a hat which of course will cancel. And these are the two derivatives in the numerator. And this ratio is evaluated at r = e.

Now this energy dependent normalization disappears from our consideration they cancel each other. And you get an expression for the logarithmic derivative.

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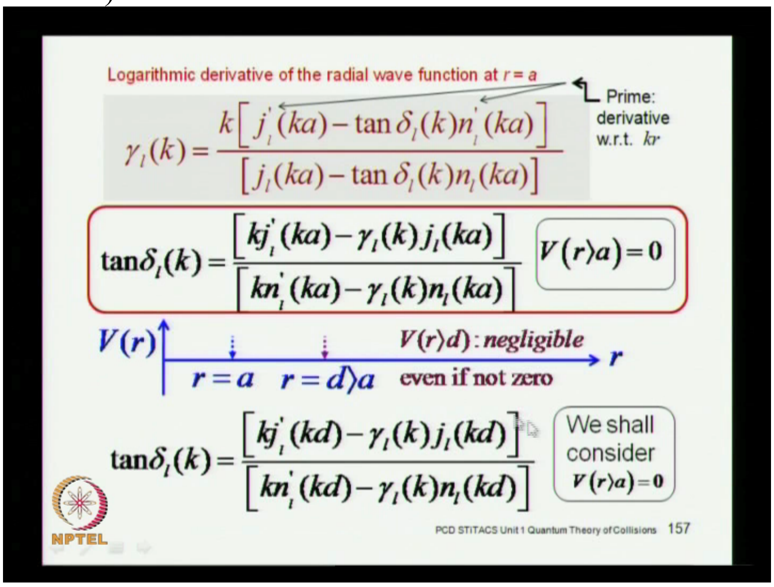

Now this expression you can invert by cross multiplying just manipulate these terms and get the expression for tangent of delta in terms of the logarithmic derivative gamma okay. We first got gamma in terms of tan delta. So, we just invert this relationship and write tan delta in terms of gamma okay. Now we are dealing with a potential which is not a strict range r greater than a is zero.

That is a strict finite range of the potential but there may be potentials which do not strictly go to zero beyond a. But they have a negligible effect outside a certain domain like r = d, beyond this even if it is not exactly zero it if it is add in is a negligible effect. Then you can still work with the relationship of this kind with a replace by d.

Because the asymptotic solution is what we have exploited here okay. So, it really does not matter but for our general consideration we will deal with those potentials which have got a strict finite range just for simplicity but actually even these potentials can be handled using similar techniques.

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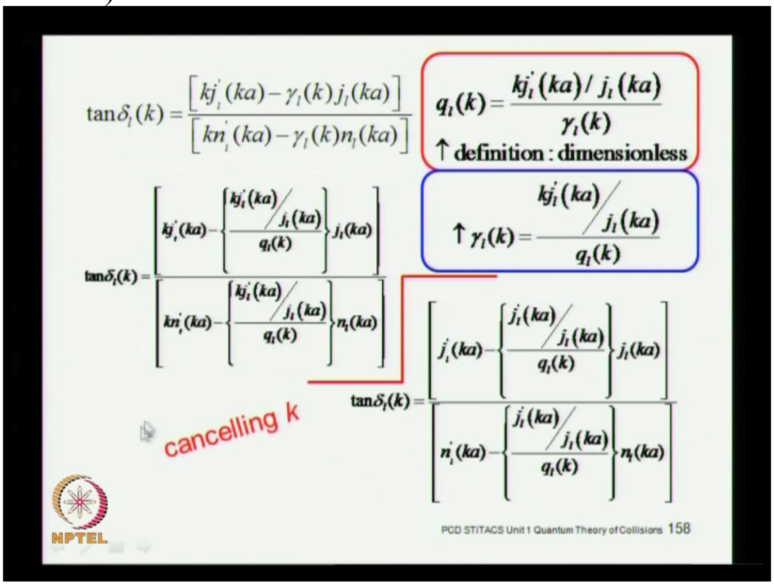

So, this is our expression for the tangent of delta and we now define a parameter called q, I am using the notation from Joe Shane's book. So, q this is the definition of q, notice that in the numerator you have got obviously a logarithmic derivative which is what you have with a new denominator also. So, this is a dimensionless quantity this is the definition of q and this is a useful parameter in scattering theory.

So, you introduce the parameter u, q using this definition and invert this to define gamma in terms of q. Now having defined gamma in terms of q, you insert this expression on the right hand side in this position for gamma which is the expression for the tangent of the phase shift. So, let us do that, so this gamma is replaced by this ratio okay. So, I have just substituted this term over here.

In the numerator there is a gamma and in the denominator also there is a gamma right. Now you find that there is a k here, there is a k here, there is a k here and there is a k here. So, k cancels everywhere and now you can write the same expression without the case okay. So, k cancels out.

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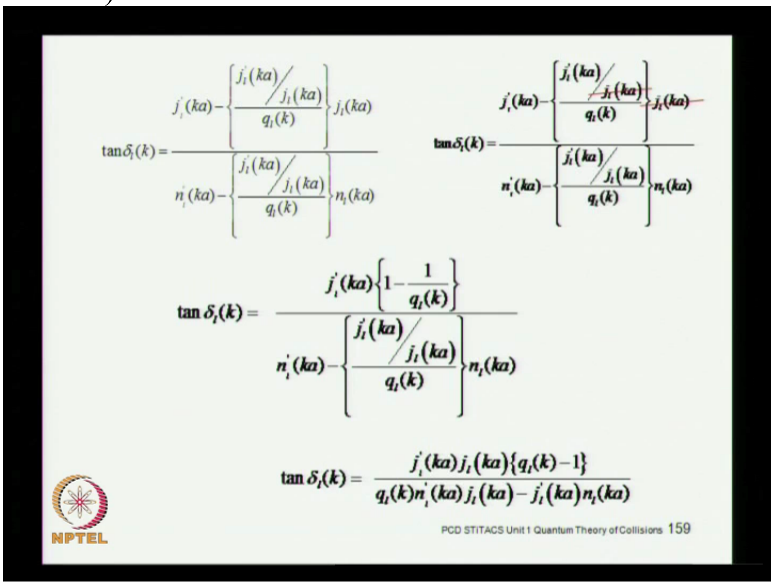

And after cancelling k notice that this Bessel function and this Bessel function will cancel each other, so jl ka and this jl ka will cancel each other. So, that leads to some simplification okay. So, this is rather straightforward manipulation of terms and you get an expression for the tangent of the phase shift in terms of this q right. So, this is jl prime ka in the first term and then there is a jl prime ka in the second term as well.

So, I take jl prime ka as a common factor and then in the numerator I have got 1 minus the inverse of the parameter q which is defined. So, this is the numerator the denominator likewise is given by this sum. Now if you again simplify this a little bit because there is a inverse q in the numerator as well as in the denominator. So, the 1 over q in the numerator can cancel the 1 over q in the denominator.

But when you do that you have to balance the second term and when you consider that balance the numerator then becomes j prime j right. And then you have got q -1 and in the denominator you have got q times n prime j - j prime n okay. And now the inverse q in the numerator on the same as the denominator cancels each other okay.

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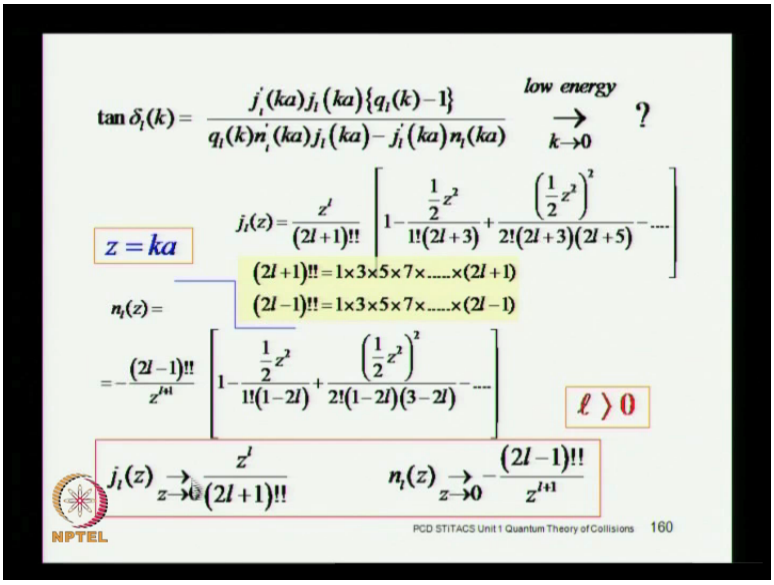

So, now we have got a fairly simple relation for the tangent of the phase shift and now you have got the Bessel function. You have got the derivative of the Bessel function and then the q parameter which has been introduced in terms of the logarithmic derivative. Now let us ask how does it behave at low energy okay. As the energy of the projectile if is diminished and in the low energy limit as k tends to 0.

What is the value of the phase shift? How does it change with energy? What is this energy dependence for small energy? That is the question we raise here, we will also later consider the high energy limit okay. So, for now we consider the low energy limits, low energy behaviour and you to make use of the expansion of the Bessel function in a power Series in z square okay.

So, the Bessel function for the quantum number l goes as z to the power l divided by this is a double factorial which is essentially a multiplication it is similar to factorial except that the even numbers are missing okay. So, only the odd numbers are multiplied in this double factorial notation and 2l + 1 is always an odd number. So, the last number up to which you carry out this multiplication is 2l + 1.

Likewise you can also define 2l - 1 which is also an odd number and you can take all the product of all the odd numbers that define a 2l-1 as well. So, you have the Bessel function which is z to the power l divided by this 2l + 1 double factorial term and then you have got a power series over here. Now z is your ka a being the range of the potential, k is coming from the momentum and it is determined by the energy.

So, in the low energy limit you are seeking the limit k tending to 0. So, obviously the leading term in this square bracket will be 1 right and you can have a similar expression for the

Neumann function which is a standard expression that you will find in any mathematics book. And you use these power series expansions for the Bessel function and Neumann function and then take the low energy limit z tending to 0.

So, the Bessel function will go as z to the l divided by this term and the Neumann function will go there is a minus sign here. So, it will go as 1 over z to the l + 1 right.

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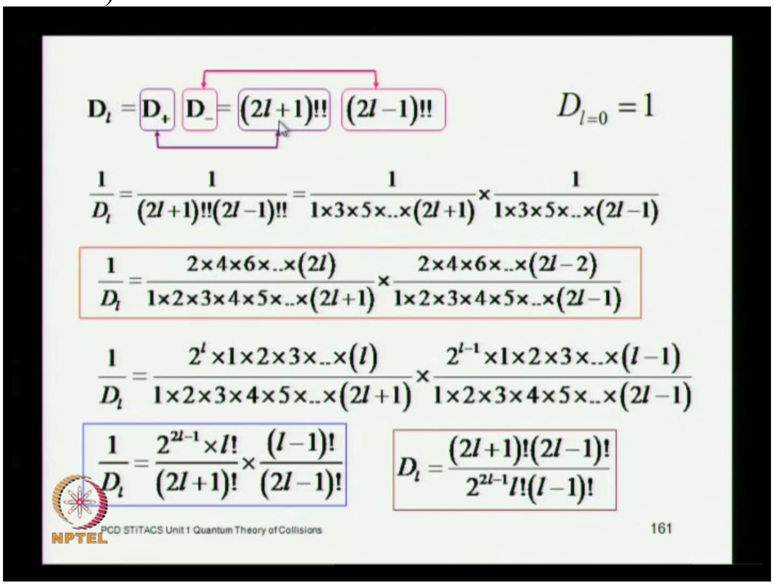

So, let us first consider l greater than zero terms, we will also consider l =0, for which this term D =1 and this is the definition of this notation in which two exclamation marks are used instead of just one to represent the product of odd numbers. And these are some alternative forms you can stick in the missing even numbers in the denominator and compensate for them by inserting them in the numerator okay.

As you can do it for the second term as well. And from this numerator 2 will always be a common factor, so you will have 2 to the power l multiplied by factorial l in the numerator. So, this is just some convenient way of writing this term this is not of much significance but only alternate and compact ways of writing this notation.

So, notice that this product of these two double factorials can be written in terms of products of these factorial terms equivalently. So, you will either see this form or this form depending on what book you are looking at. But it is essentially the same term okay.

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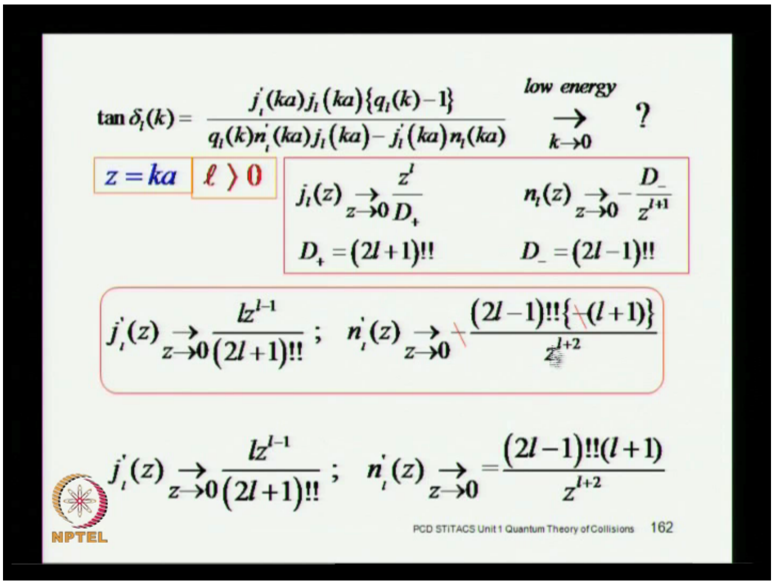

So, this is just a matter of notation and we come back to our analysis of the low energy behaviour of the tangent of the phase shift. And we have found that this low energy behaviour of the Bessel function goes as z to the power l and of the Neumann function is goes as 1 over z to the power l + 1.

So, now to get the behaviour of the phase shift at low energy you need the Bessel function here and also here and then you need the Neumann function here and you need the derivative of the Neumann function here. So, you need not only the Bessel functions that the Neumann functions you also need the derivatives and these are the derivatives of the Bessell function and Neumenn function in the small energy region as k tends to zero.

So, it is just the derivative of z to the l which is lz to the l - 1 and likewise over here you will get 1 over z to the l + 2. So, there is a minus sign here and a minus sign here so that can be struck off. And these are the derivatives you get for the Bessel function and the Neumann functions. So, mind you this is there is a prime here which denotes a derivative.

So, these are the derivatives of the Bessel function and the Neumann function. And these approximate derivatives which you have on the right hand side which are reasonable approximation at low energy. They can be used over here with this expression for the tangent of the phase shift to examine the low energy behaviour.

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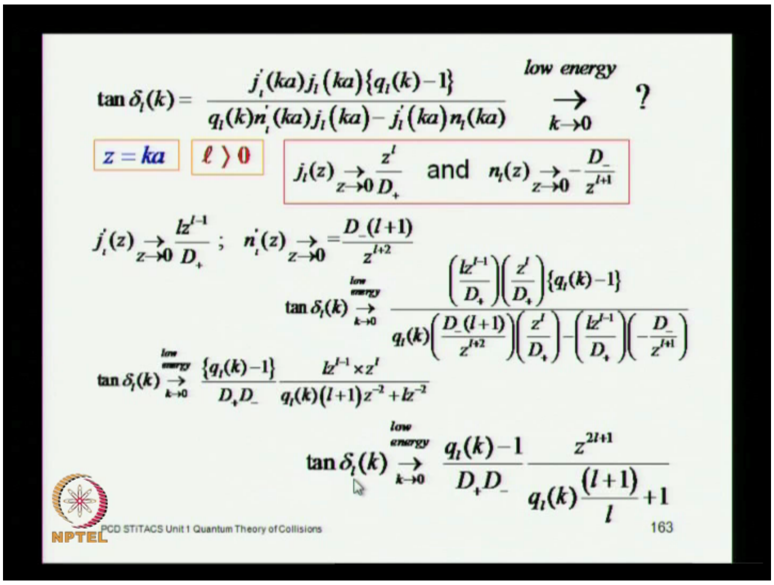

So, let us put those terms in, now this is what you get. So, this is j prime, so j prime is lzl to the -1 over D+, this is j the Bessel function which goes as z to the l over D+. So, you got 1 over D+ square in the numerator and in the denominator if you plug in all the terms you put the n prime the j and the j prime and the end you get 1 over D+ over here okay. So, 1 over D+ square in the numerator and 1 over D+ in the denominator.

You will be left with only 1 power of D + and the denominator over all right. And then you also have a D- overall in the denominator. So, you get product of D+ and D- in the denominator. In the numerator you have got this q - 1 term which remains as it is. Then you got a product of lz to the power -1 and z to the power l right. And then you have got the rest of the terms over here which is q times l + 1 is coming from here, z to the power l.

And then this, z to the power l, and you also have an lz to the power l -1 over z to the power l +1 over here. So you can take z to the power l from the denominator to the numerator z to the power -l goes as z to the power +l in the numerator and then you are left with z to the power -2 in the denominator okay. So, this is just simple rearrangement of the powers of z. Z in our case is of course ka, so we know that the energy is a parameter there.

So, this is the expression that you get notice that this phase shift goes as the 2l + 1 power of ka okay. That is the result which is emerging from this and we will see it explicitly.
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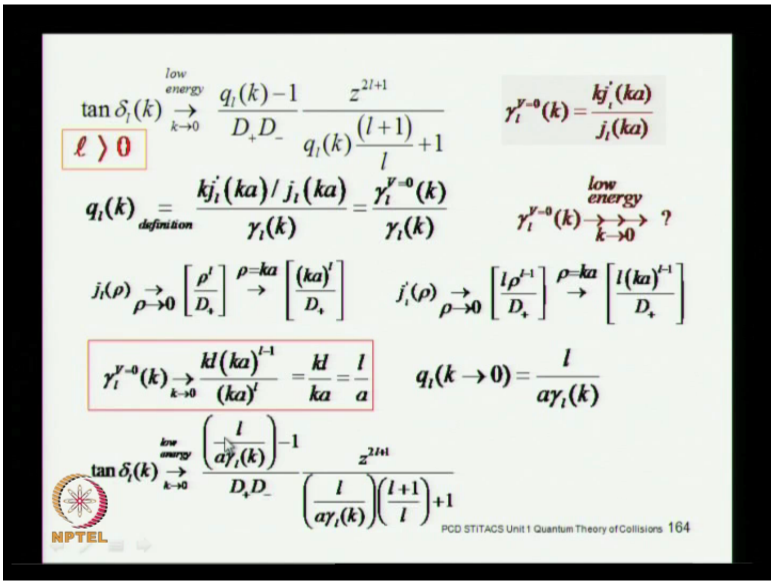

So, this goes as z to the power 2l +1. And then you have got the remaining terms over here. Now what is q? q Was defined as the ratio of these two logarithmic derivatives the numerator is the logarithmic derivative for the free particle. The denominator is the logarithmic derivative for the case of interest in which you have got a certain target scattering potential.

So, this is the logarithmic derivative for v = 0, further and then you can ask what is the value of this as k tends to 0 okay. This is the free particle logarithmic derivative at an arbitrary energy and it will have a certain approximate value as a tends to 0 as k tends to 0. So, this you can determine by taking the logarithmic derivative corresponding to the free particle which is the Bessel function and its derivative.

And you take the Bessel function you take the derivative of the Bessel function and you find that the logarithmic derivative for the free particle goes as l over a okay, that is the leading term okay. There are other terms that we can consider some of them as we need them. But this is the leading term so the leading term goes as l over a and this means that q goes as l over a.

And it is multiplied by 1 over gamma because that is the definition of q right. So, we can put this value of q which is l over a gamma over here this is q. And this q is replaced by l over a gamma rest of the terms are the same which is l + 1 over l + 1 you have got z to the power 2l + 1. And then you have got the coefficient q -1 but q is l or a gamma. So, that is what is used here right.

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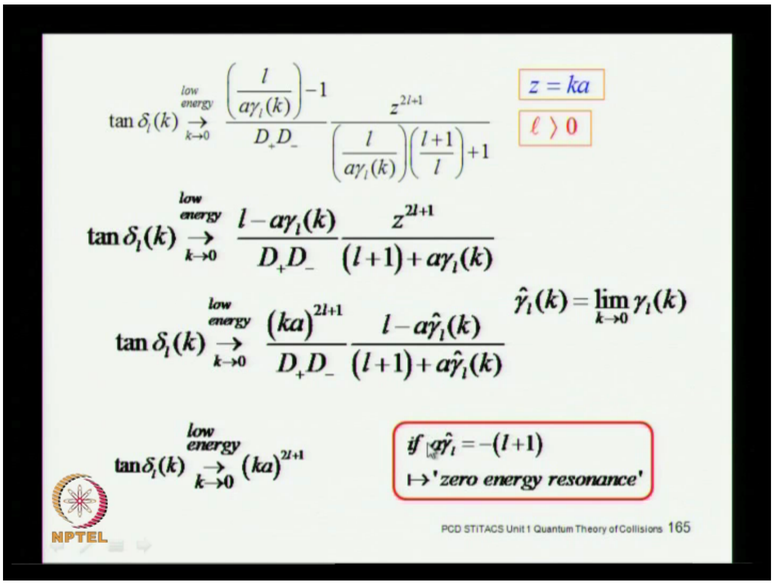

So, now let us simplify this a little bit. So, this is l over a gamma -1, so you will get l - a gamma over a gamma right. And you do the same in the denominator and then you cancel the a gamma and then the remaining terms which survive are l - a gamma over D + D minus product. And then z to the power 2l +1 and in the denominator what you have this l cancels this l.

So, you have got l + 1 + this a gamma would have multiplied this one. So, that is the term which comes here and essentially we need the limit of gamma as k tends to 0, so this limit is indicated by gamma carrot like putting a little tiny hat on top of gamma. So, this is the low energy limit of the logarithmic derivative which is the term of interest. So, the tangent of the phase shift has a low energy behaviour k tending to zero behaviour.

Which is given by ka to the power 2l + 1, l – a, gamma this is gamma carrot which is the low energy limit of the logarithmic derivative and l +1 +a gamma carrot. So, this is the overall conclusion. That the low energy phase shift goes as k to the power 2l + 1 that is the overall conclusion which comes other than you know multiplying factors and so on.

But this is the dominant story which is emerging mind you however that there is a denominator here l + 1 + a gamma and it could happen in some particular case depending on a value of l. Because in the partial wave analysis you have got all values of l, so the denominator is not just a single value you have got the similar term for each partial wave.

So, for some particular partial wave for some particular quantum number l and if it happens for that quantum number then you have to consider this term carefully that if this term happens to be equal to minus of l + 1 then this term is going to blow up and you will have some sort of a zero energy resonance in this case have that something that we might want to consider.

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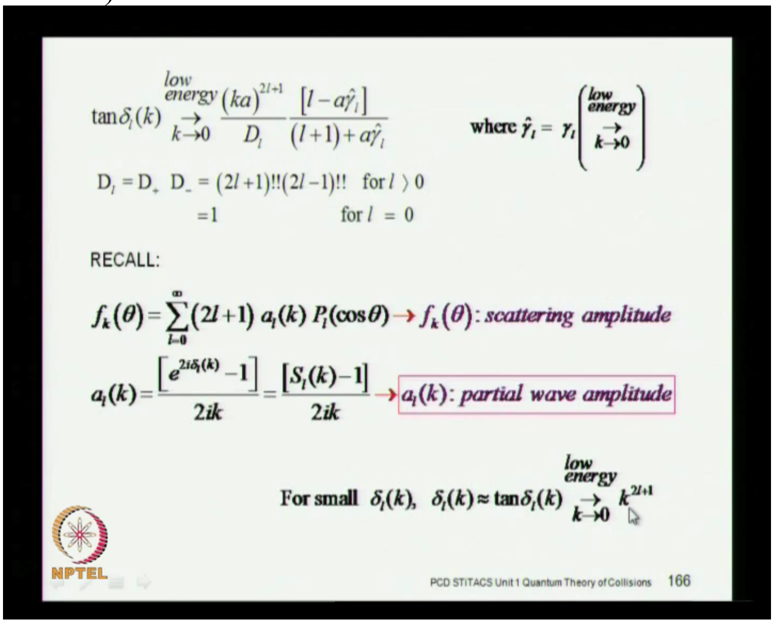

So, for the moment let us consider these situations which is a non resonant phenomena. And we will see what consequence it has on the scattering amplitude and the partial wave amplitude. The partial wave amplitude is what goes into the scattering amplitude the scattering amplitude this is the Faxen Holtzmark's you know resolution of the scattering amplitude in partial waves partial wave decomposition of the scattering amplitude okay.

So, this has got the S matrix element which is e to the 2i delta and let us consider as we have been doing in analysis small tiny phase shifts. For which delta will be almost equal to sine delta which is almost equal to tan delta okay. So, for small angles the angle itself and the sign and the tangents they are nearly equal if you take the leading term in the corresponding power series of the sine and the tangent function.

So, tan delta or the phase shift itself goes as 2l + 1, as we have seen because that is how the tangent goes to which the phase shift itself is very, very similar.

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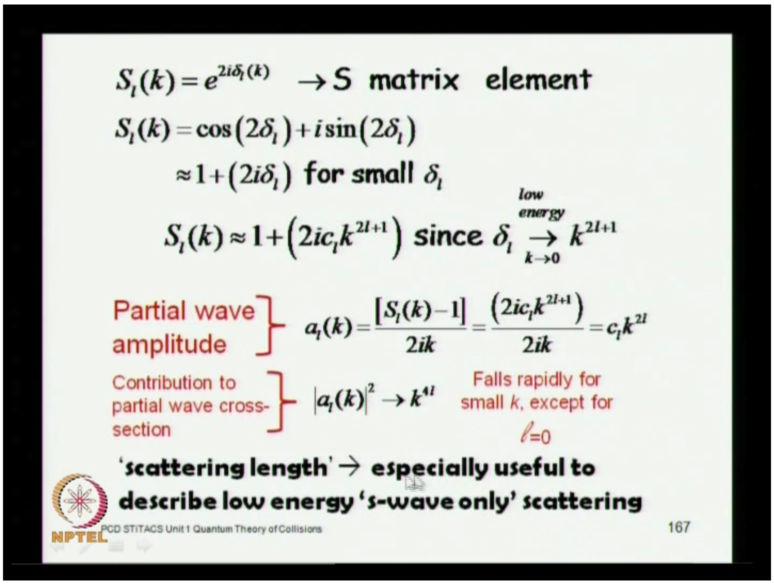

And this is the S matrix element. So, this is cosine 2 delta + i sine 2 delta which for a small angle the cosine of this is nearly equal to 1 and the sine of this angle is nearly equal to 2 delta itself right. So, you get 1 +2i delta for small delta. Which means that the S matrix element is nearly equal to 1 + this 2i times the phase shift.

And this phase shift we know goes as the 2l + 1 power of k, other than some multiplying constants which I have written as c with a subscript l. So, this is the overall behaviour low energy behaviour of the phase shift, so the partial wave amplitude so you have to subtract from this S matrix element 1.

So, that this one will go and then this 2ick to the power 2l + 1 is divided by 2ik, so you get the partial wave amplitude goes as k to the power 2l + 1 because 2l + 1 is divided by 1 power of k over here, so this goes as k to the power 2l. So, the modulus square will go as 4l and as l increases as energy decreases this will go very rapidly to zero okay.

Because you are taking the fourth power and not just fourth power if l =1, you are taking the 4th power, if l =2 you are taking the 8th power, if l =3 you are taking the 12th power of k. So, it goes to 0, very rapidly. And the leading term will of course come from l = 0 which is why the S wave scattering is of so much importance this hangs well with our understanding of the centrifugal barrier and everything that we have learnt about the partial wave analysis.

That you do not really have to consider higher partial needs and it is the S wave scattering which is of most importance. But then of course other terms are also contributing and the S wave scattering does play a very important role. And for the S wave scattering it is very useful to define a parameter which is called as the scattering length which I will now define. It is particularly useful in low energy scattering phenomena.

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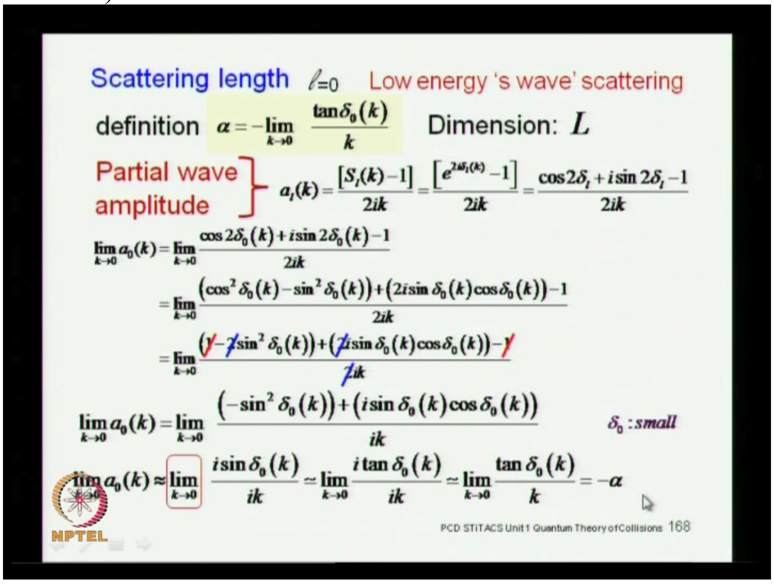

So, let us define the scattering length for the s wave and this is the definition of the scattering length alpha notice that it goes as 1 over k, so it will have the dimensions of length which is why it is the length okay and this is the definition of scattering length. The partial wave amplitude we have seen is given by this expression.

And if you now take the low energy limit of this partial wave amplitude, take this limit as k tending to 0 then you have this cancellation of 1 over here, this cos square delta is written as you know you have got all of these sine functions and so on. So, if you just manipulate those trigonometries carefully then this one cancels and essentially then these two factors, two cancels and you are left with sine square delta -sine square delta over here.

But then again you deal with small delta for which sine square delta will be ignorable delta square is very small and cosine delta zero will be nearly equal to 1. So, this whole expression reduces rather simply to this i sine delta over ik. Because cos delta is nearly equal to 1 sine square delta can be dropped okay, it is a small quantity and you cancel the i over here and this by definition is the scattering length.

So the scattering length or rather it is negative is what gives you the partial wave amplitude in the low energy limit okay. That is why it is so important.
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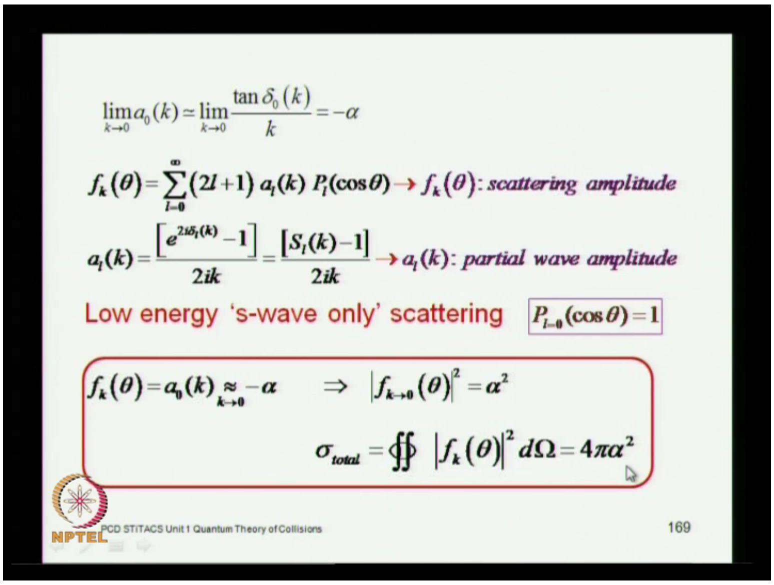

Now once you have the partial wave amplitude you can get the scattering amplitude. And what is the scattering amplitude? If l =0, alone is contributing then this 2l + 1 = 1, al of k emerges in terms of the scattering length Pl of cos theta for l = 0 is just equal to 1 right. So, essentially you get the scattering amplitude equal to the partial wave amplitude which is equal to the scattering length with a minus sign.

But you are anyway interested in the square of this, so that gives you alpha square. And this of course is the differential cross section d sigma by d omega okay. This is the differential scattering cross-section d sigma by d omega if you integrate it over all the angles. You will get the total scattering cross section which will be just the total solid angle which is 4pi times alpha square which of course will have dimensions of length square.

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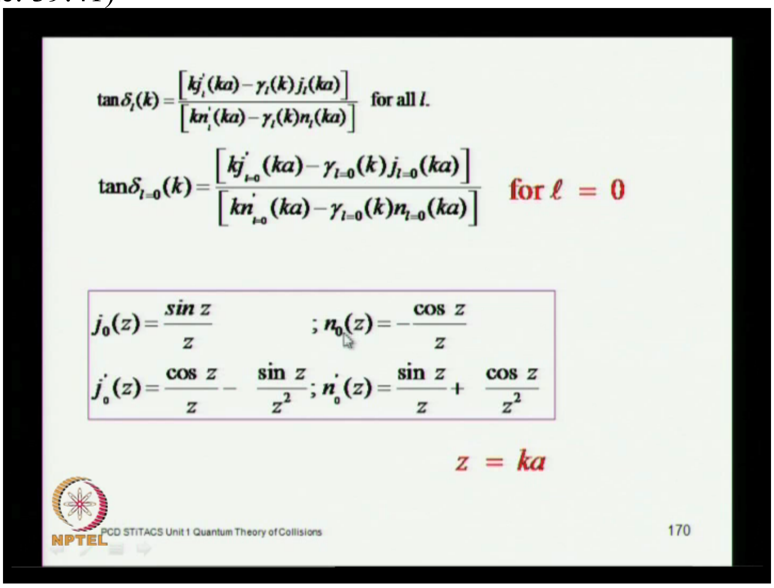

So that is what we get and let us look at this expression for l = 0, for l greater than 0, we have always already looked at the expression for tan delta. We have seen that it goes as k to the power 2l + 1. Now let us see what it does for l = 0. So, for l = 0, you have explicit expressions for the Bessel functions which are exact okay. And you use these expressions for l =0, so the Bessel function is sine z by z, the Nuemann function is - cosine z by z. So, you can take the derivatives okay.

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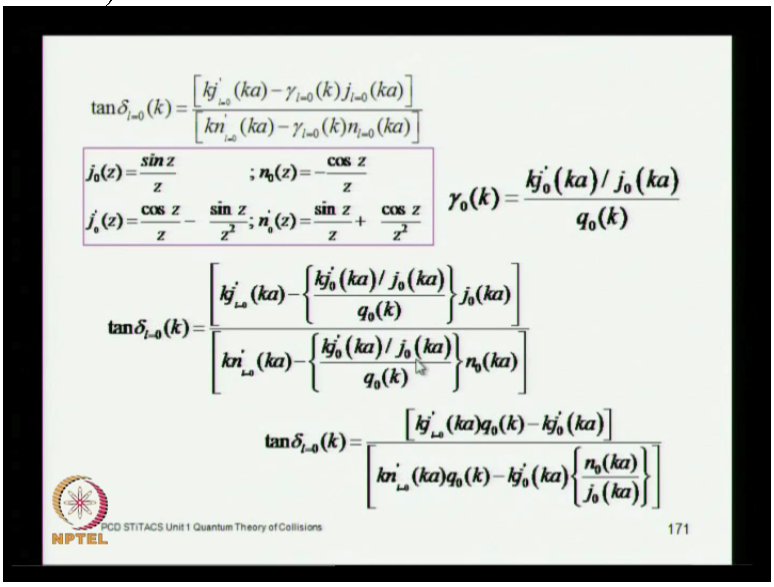

Put z = ka and then put all those terms in this expression for the tangent of the phase shift. And once you put all of these expressions over here gamma of course has to be determined this can also be determined easily in terms of the Bessel function and its derivative in terms of the parameter q.

So, q is going to appear in this expression now because we are expressing the logarithmic derivative in terms of q. So, this is just a simplification with this gamma in the numerator and in the denominator replaced by this ratio which is defined in terms of q. So, you simplify this expression a little bit multiplied by q0.

So, you get kj prime times q0 in the first term. Then you have got the numerator of the second term but this j0 ka cancels this, j0 ka so there is some simplification coming from there you have only kj0 prime which is what you have over here. You do the same thing with the denominator.

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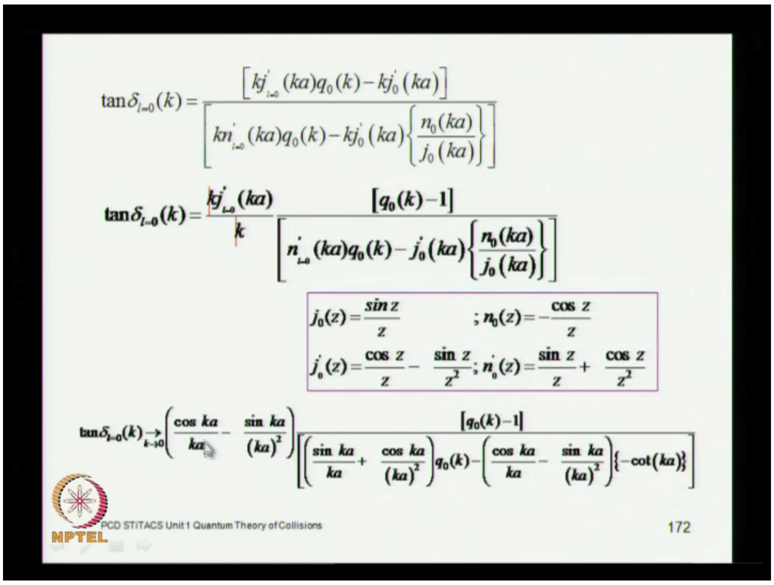

And you have a rather straightforward expression the tangent of the phase shift. So this is the derivative of the Bessel function okay. Now there is a k here and there is a k here so you will be able to cancel them. And now the derivative of the functions are also known because you have the explicit form of the Bessel function as well as the Neumann function okay.

So, what 1 over ka and 1 over ka square in all the terms either 1 over ka or 1 over ka square in all the terms this is in the numerator this is you have got some other things in the denominator.

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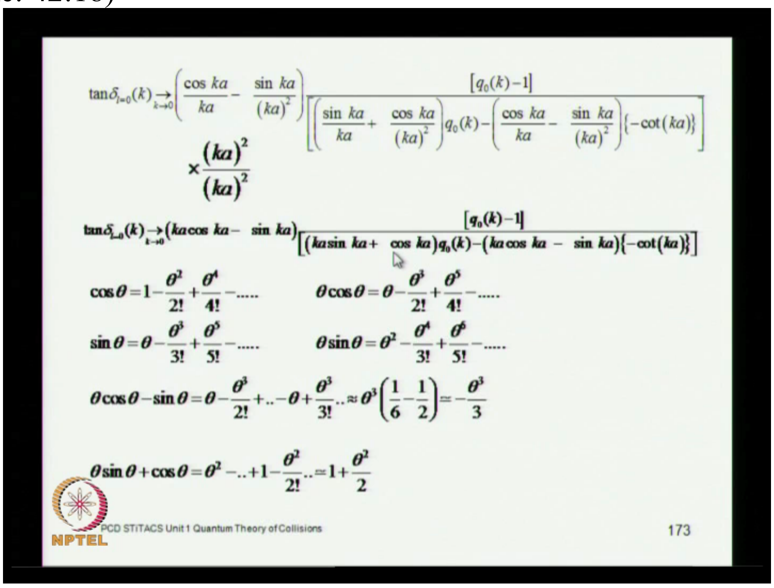

So, it becomes useful to multiply and divide by ka square okay and that will give you a rather simple expression here. And here you have got expression like theta cos theta - sine theta, theta being ka and here you have got theta sine theta + cos theta okay. And here again you have got theta cos theta - sine theta but we have the power series expansions for sine theta as well as for cos theta.

So, you using those you can get the expansions for theta sine theta and for theta cos theta. And plug those expansions in and then take the leading term okay. So, these are the expansions for the cosine and the sine functions. So, these are the expansions for theta cos theta and theta sine theta you just multiply each term by theta. In these expressions and then here you need theta cos theta - sine theta this is where you have theta cos theta - sine theta.

So, that will have this theta cancels this theta this one is with a minus sign and this is with the plus sign okay. And the leading term in this goes as the cube of theta with a minus sign. So, this goes as - theta cube over 3. Now this is for theta cos theta - sine theta you do the same for theta sine theta plus cos theta over here and this goes as 1 + theta square by 2.

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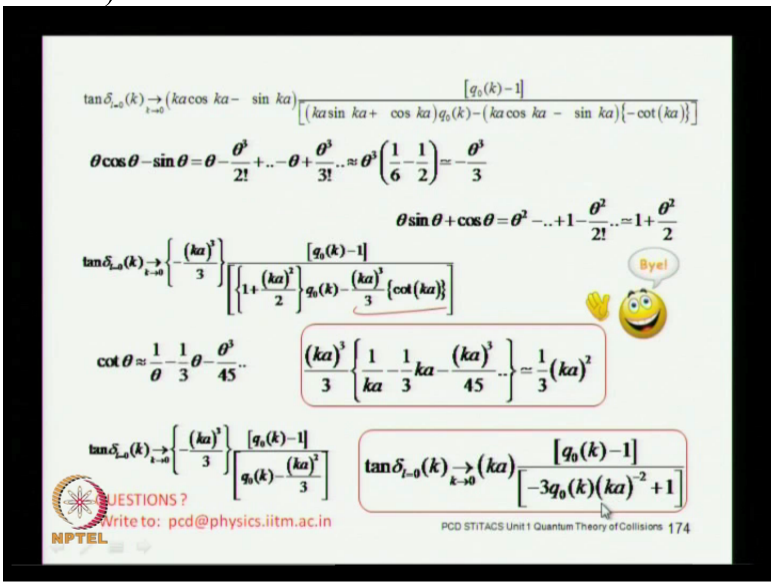

So you can insert these approximate expressions retain the leading terms. The leading term here is - theta cube over 3 keep the leading terms over here. And the cotangent can also be expressed in the series. And then you have to multiply the power series for cotangent with a cube of theta okay and that helps. And then once you take care of this so when you multiply this with the cube of theta you get square of theta with 1 over 3 factor okay.

So, to keep track of all the signs and the factors accordingly and now that gives you an overall expression for the tangent of delta over here, so got ka cube when you got a ka square in the denominator okay. So, you can extract the ka square as a common factor in the denominator.

So, this term becomes -3q0 times ka to the power -2 and this kaq is divided by ka square so you get one power of ka. So, this is now in a form similar to the form we had for l greater than 0 okay. So, both the forms whether it is l = 0 or l is greater than 0 you will get an expression for the tangent of the phase shift in very similar form.

And we will continue from this point in the next class. So, thank you very much, if there is any question I will be happy to take otherwise goodbye for today.