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

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**Lecture 07**
**Unitarity of the Scattering Operator**

Greetings, we will continue our discussion on the partial wave analysis for scattering are there are two questions we will take up today. One is when you consider the resolution of a plane wave in partial components. You have a summation over the orbital angular momentum quantum number l going from zero all the way through infinity.

And if you really want to do a calculation with all these partial waves with infinite terms you will never really finish it. So, is there any maximum angular momentum quantum number up to which you need to consider the terms that is one question that we will take up? And fortunately there is in most of the situations although there are some exceptions also.

The other question which we will take up for today's discussion is the Unitarity of the scattering operator and we have mentioned the optical theorem, we have considered the optical theorem on the basis of the conservation of flux, the equation of continuity that we have considered earlier.

So, you already have the result for the optical theorem but we will show that the theorem holds it is a very powerful theorem and it has got a much more general credibility than what we considered earlier. And it is connected with certain properties of the scattering operator the scattering matrix which is specifically the Unitarity of the scattering operator.

So, I will introduce some of these things today. Most of this discussion is from Landau and Lifshitz book for today.
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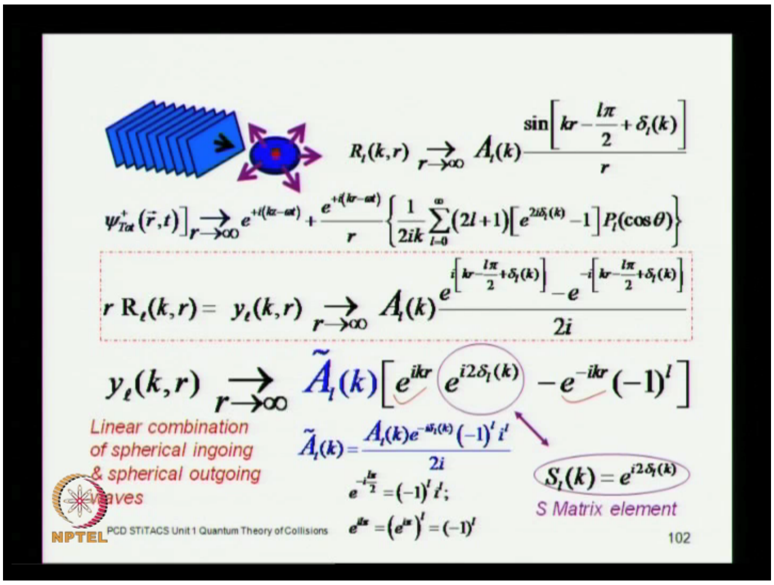


So, let me quickly recapitulate some of the main results for the partial wave analysis. So, you have got the asymptotic form of the radial solution in which you now have a phase shift which is coming as a result of the potential. We have therefore the outgoing wave boundary condition solution indicated by this plus symbol on top.

And this outgoing wave boundary condition in the asymptotic region has got this form. So, you have got an incident plane wave and a scattered outgoing wave which is scaled by the scattering amplitude which is in this curly bracket. So, if you multiply this radial function by this little r, you get a function called little y.

And y has got this asymptotic form and you can write, rewrite this y you can extract this e to the -il pi by 2 and e to the i delta lk as constants, extract them. So you get a different constant and then you get e to the i twice delta -e to the - ik r times -1 to the l, which is coming from this e to the il pi.

So, we have seen these equivalent forms and you notice that in this last expression you have written this radial function or what is r times the radial function as a superposition of spherical outgoing waves and spherical in going waves okay. Now this is the superposition of ingoing and outgoing spherical waves. In which this outgoing wave is scaled by the scattering phase shift.

There is an e to the i delta here, in this A tilde as well by it does not matter that is outside and that is a part of the common normalization that can be taken care of. So, the main function which is in this rectangular bracket is a linear superposition of spherical outgoing wave and in going wave. In which the outgoing wave is scaled by this e to the i 2delta and this is sometimes referred to as the S matrix element.

As to why it is referred to as S matrix element? What is the S matrix? What is the scattering operator? These are the things that I am going to introduce today.

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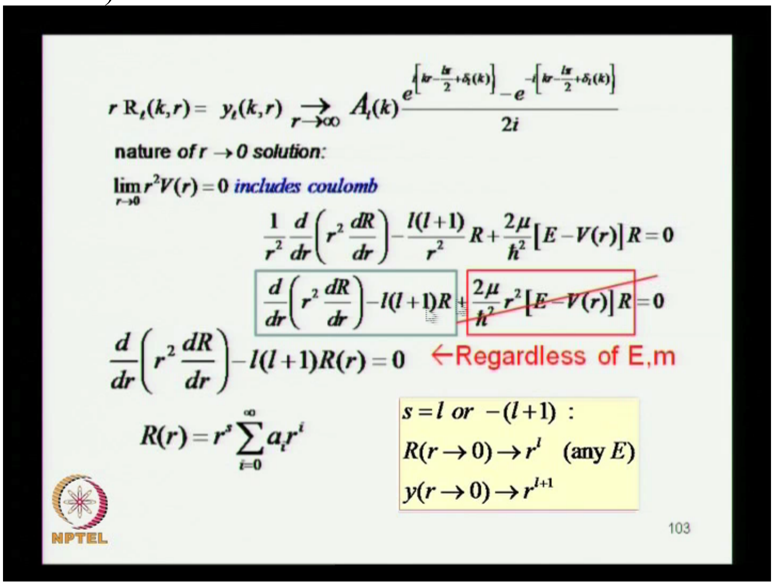


So, this is the function that we have been talking about. Let us look at the general nature of the solutions, first the r tending to zero region, it is always a good idea to look at the form of the wave function in different limiting you know conditions. So, r tending to zero and r tending to infinity are the two regions of particular interest.

And we considered a potential which goes to 0 as r square Vr. So, this will include Coulomb because Coulomb goes as 1 over r, so this will be applicable to the Coulomb as well and for a potential of this kind you can write the radial form of the Schrodinger equation. In which you have separated the angular part.

In these two equivalent forms and when r square V goes to 0, so r square into e already goes to 0, no matter what value of e, but r square V also goes to 0 which means that you can throw off this term. So far as the major consideration with respect to the nature of the solution as r tends to 0 is concerned.

And the rest of the differential equation is now a simple one in which you have got only these two terms equal to 0. So, this is the form of the differential equation which is of importance in the smaller region as r tends to 0 and this has got its validity independent of the energy. Because energy has gone off the mass mu has also gone off, so it really does not matter.

And this is the differential equation that you have to solve. And if you attempt a power series solution for this then you have got two solutions one of which is regular at the origin which goes as r to the power l and the corresponding solution to this function goes as r to the power l +1, which is r times this. So, it goes as r to the power l +1.

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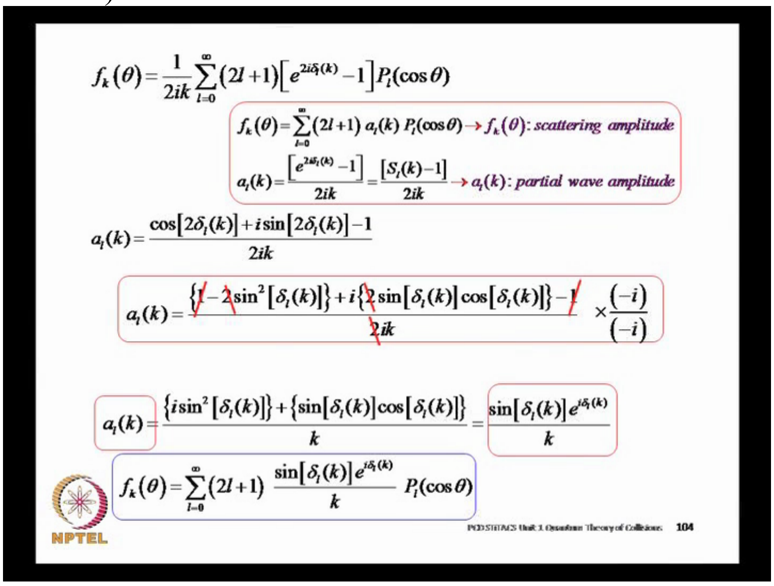


This is the expression for the scattering amplitude as we have got. Now you can write this scattering amplitude, you have got a 2l + 1 factor here and a Pl cos theta and this term in the rectangular bracket is what i have called as alk. This is sometimes called is a partial wave amplitude. So, the partial wave amplitude is different from the scattering amplitude this is a, this is f and this there is a simple relationship between the two.

This, a includes this 1 over 2ik factor okay, so this S matrix element -1 divided by 2ik is the partial wave amplitude. And if you look at this partial wave amplitude now which is e to the 2i delta -1, so it is cos 2 delta - i sine 2 delta -1 and you can expand this 2 delta and sine cos 2 delta and sine 2 delta using usual trigonometric identities and find that this one factor cancels this one at the end.

And then you are left with a factor to a factor 2 and a factor 2 in the denominator. So, all the, these factors cancel out. And the rest of the term you can multiply and divide by –i, like this so that this partial wave amplitude is once you multiply the numerator by –i, so you get minus into minus plus sign and then i times sine square 2delta.

And from the second term you get a =1 because you get a minus i into i which is i square - i square. So, you get a + sign and then you have sine delta times cosine delta. So, if you extract sine delta is common in these two terms then you get sine delta e to the i delta by k right, so that is your common factor. Now this is your expression for the scattering amplitude.

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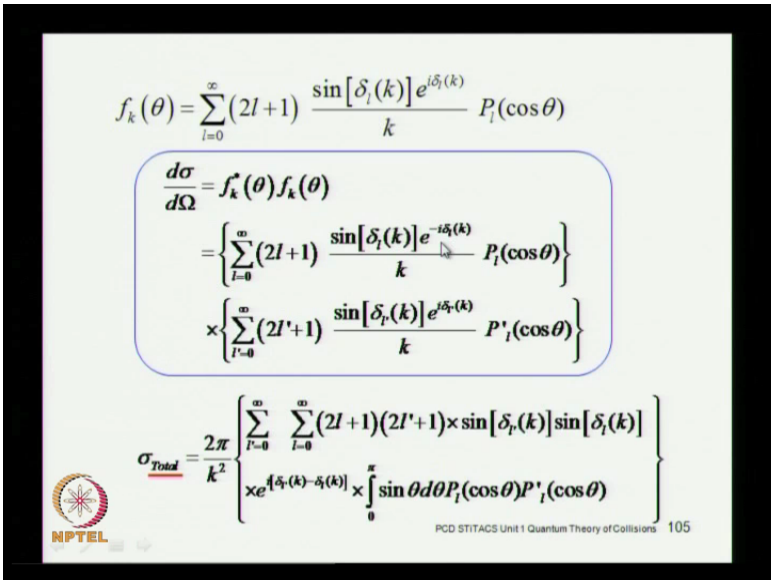


Now if you look at the scattering amplitude once again you can use it to get the differential cross section which is f star f. Now f star is the complex conjugate of this, so you have got a partial wave expansion in l = 0 through infinity. And then you get the complex conjugate of this, so e to the i delta becomes e to the -i delta, rest of the terms are real. And here you have got in f, a similar partial wave expansion.

But now the dummy index is l prime okay, so I have used a different dummy index for f and a different dummy index for f star. So, now you have the total cross section which will be an integral of d sigma by d omega over all the angles so there will be an integral over the azimuthal angle Phi that will give you a factor of 2 pi. So, that 2 pi is here, the 1 over k and this 1 over k gives you 1 over k square.

So you have got 2 pi over k square and then you have the rest of the terms which is the double summation over l prime and l you have got a 2l + 1 coming here and 2l prime + 1 coming here. You have got the product of the two sine functions sine delta and sine delta l prime.

So, the sine delta l prime and sine delta l right, and then you have got the difference in the phase shifts e to the power this is + i delta l prime and this is e to the -i delta l. So, that difference gives you e to the i delta l prime - delta l and then you have got the integral over the polar coordinate theta going from 0 to pi sine theta d theta. And then you have got the product of these two Legendre polynomials right.

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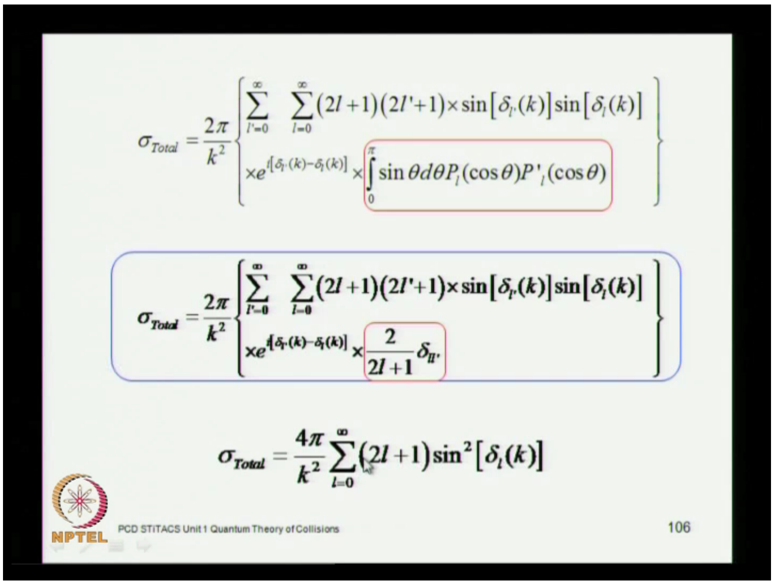


So, let us write this expression which is the product of the legendre polynomials and you have got an integral over here. And you can obviously use the orthogonality property of the legendary polynomials here. What does that give you? You get ll prime and you get a factor of 2 over 2l + 1.

So, now you have got two summations over l prime and l, one of which will contract under this kronecker delta. This 1 over 2l + 1, will cancel this 2l + 1, there is a factor 2 here, so this 2 into 2pi will give you 4pi and you have got 4pi over k square. There is now a single summation l going from 0 through infinity.

Then you have got the product of these two sine functions but now l and l prime are the same so you get a sine square delta l. And then this e to the phase factor gives your unity because the two phases become equal when l = l prime, no matter what that phase shift is okay. So, get the total cross section to be given by a sum over all these partial wave contributions 2l + 1 sine square delta l.

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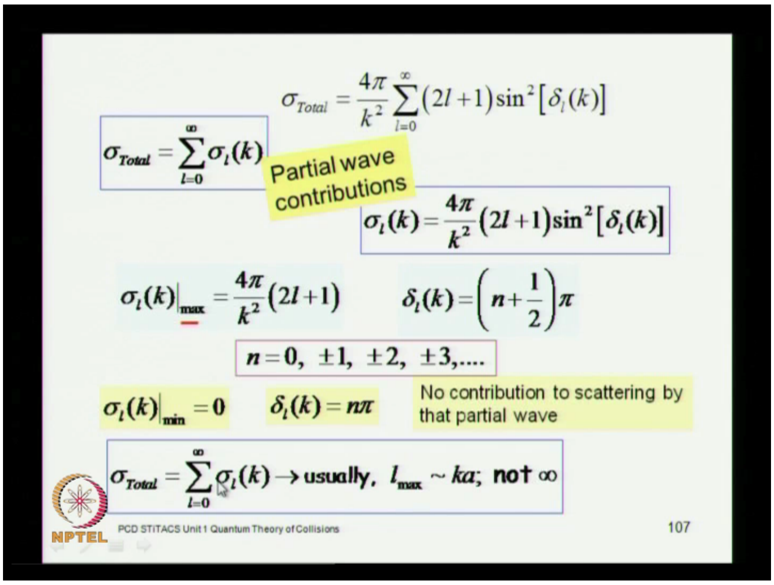


So, this is your total cross section. Now you can write this as if, a sum of partial cross sections for each partial waves each lth partial wave. In which the partial cross section for the lth partial wave will be 4pi over k square 2l + 1 sine square delta l. And notice that this can be 0 if sine delta is 0 okay, that depends on the phase shift. And its maximum value is 4pi by k square times 2l + 1, when sine delta is equal to + or - 1 okay.

So, the maximum value of the lth partial wave cross section is 4pi over k square times 2l + 1, this is what you will get when delta l the phase shift is n + half times pi, when n is either 0 or + or – 1, + or -2 and so on right. So, this is what you will get for the maximum contribution of the lth partial wave. It can also vanish when this phase shift goes to an integral multiple of pi because the sine of that angle will go to 0.

So, there will be no contribution to scattering coming from that particular partial wave okay. Does it mean that there is no contribution to the total scattering cross section because there may be contributions from other partial ways? But for this particular partial wave namely the lth is partial wave the contribution could vanish.

So, now the total cross section is the sum of all the contributions from different partial waves and this requires you to sum over infinite terms. But thankfully you do not have to go all the way to infinity otherwise you will never finish the calculation okay. There is a certain maximum beyond which you really do not have to carry out the calculation okay, typically although there are some exceptions.

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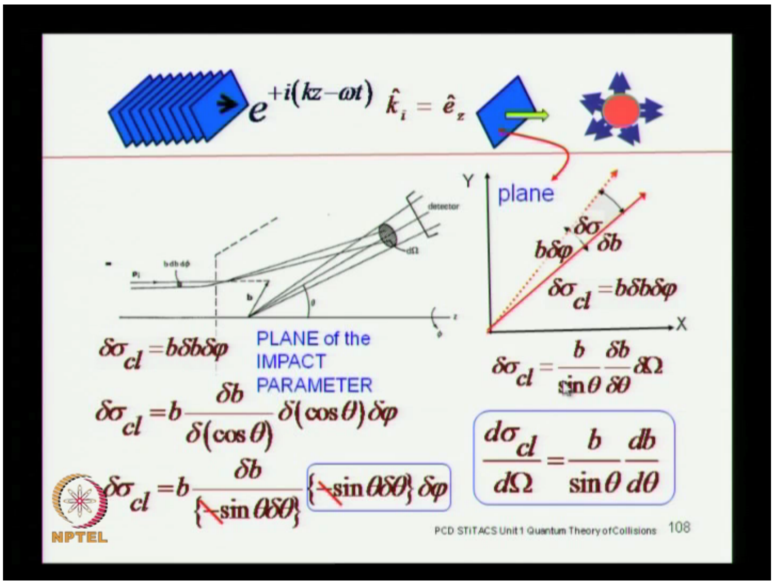


So, this is the picture which requires us to consider the resolution of the plane wave in infinite partial waves. And if you look at the plane of the impact parameter okay, you have got the incident beam coming from the left and then there is the plane of incidence; is this orthogonal to the direction of incidence.

This is the plane of the impact parameter right, impact parameter is the direct least distance between the incoming direction and the center of the scattering right, that is the impact parameter. So, what I am going to do is to consider a semi classical argument to indicate that you will have a maximum l quantum number beyond which you really do not have to consider the terms in partial wave analysis.

So, think of a semi classical argument and you have this picture of the impact parameter. So, this is a radial distance from this axis and this impact parameter b, this is completely in this plane which is perpendicular to the direction of incidence. Now, this is the plane which is perpendicular to the incident plane right.

So this distance is b, if you consider the azimuthal displacement about the axis of symmetry then a tiny as azimuthal displacement delta Phi will give you an arc which is p delta Phi and a tiny incremental increase in the impact parameter will give you delta b. So, that this cross section is delta sigma which is the product of delta p and p delta Phi.

So, this is the cross section this is the differential tiny cross section element which the target will pose to the incident beam. So, the incident beam is coming and then in that infinitesimal delta phi angle in the plane of the impact parameter you will have a little bit of you know obstruction. So, what is the obstruction provided by the target that is what this question is about right.

Whole issue of scattering is what is obstruction? Which is provided to the incident beam by the scattering target? It is this abstraction which results in the phase shift delta. So, this is a semi classical kind of an argument and you find that this differential cross section delta sigma in this tiny elemental area is b delta b times delta Phi right.

So, let us look at this differential cross section which is a cross section element which is delta sigma which is b delta delta Phi and you can write this as delta b over delta cosine theta because this theta is the polar angle with respect to the direction of incidence. The reference direction for the polar axis is the direction of incidence. So, theta is this angle and a little bit variation in theta will cause a change in this term.

So, delta cos theta, I have essentially multiplied and divided this term by delta cos theta and then this delta Phi is here. So, this is essentially b delta b delta Phi right. What is delta cos theta? The radiation is because of theta, so it is -sine theta delta theta right. So, let us write this, so this is -sine theta delta theta in both the terms here, in the numerator here, in the denominator and you strike out the - sign.

And then here the sine theta delta theta delta Phi is nothing but the solid angle delta omega right. So, your cross section area delta sigma becomes b over sine theta, that is this b over this sine theta and then you have got delta b over this delta theta. And then you have got the solid angle delta omega okay.

Now look at this expression this is going to give us a very simple analysis. So, if you divide both sides by delta omega and take the limit delta omega going to zero you get d sigma by d omega which is the differential cross section in the semi classical approximation. And this becomes b over sine theta db by d theta right.

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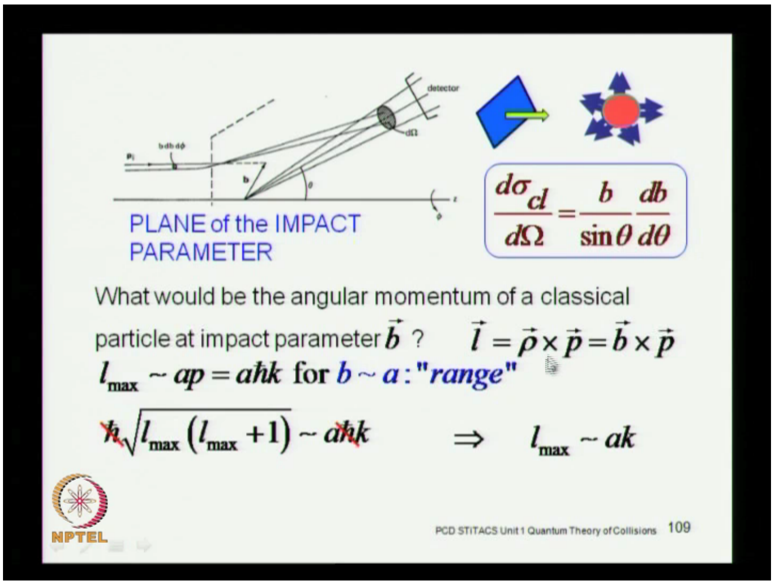


So, this is now, let us have a look at this plane of the impact parameter again and this is your expression that you have determined which is d sigma by d omega which goes as db over d theta. And now let us ask this question what would be the angular momentum of a classical particle at an impact parameter b? Okay this is the angular momentum about the axis of course right.

So, what will be this angular momentum this will be Rho cross pr cross p is the angular momentum right, the classical angular momentum. So, this is a Rho cross p where Rho is the radial vector from the axis, so it is rho cross p. But Rho is nothing but the impact parameter, so it is b cross p right. So, this is the classical angular momentum and the maximum value that this angular momentum will have is when this is maximum.

So, when b is roughly equal to the range of the potential okay. If the potential has got a certain range beyond which it will not pose any obstruction to the incident beam. If that is a finite range of the potential and all physical potentials will have a certain physical range they will of course go to zero at infinity nothing will have a effect at infinite distance. And this, the effect of any potential will go on diminishing, the farther you go away from it.

So, let us say that there is some effective range; it need not be very straight. This is an order of magnitude estimate, so you are not looking at very sharp cut offs. But the general idea that the potential will have a certain range beyond which it will not offer any obstruction to the incident V.

And if that range is equal to a then the maximum angular momentum here will be a into p, which is here right and p is h cross k right, momentum is h cross k and this is what gives you the maximum angular momentum. Now what is this equal to this angular momentum on the left hand side? Now let us bring in a little bit of quantum mechanics. So, this is like old quantum theory okay.

Mix a little bit of classical mechanics with a little bit of quantum mechanics okay and the angular momentum in quantum mechanics goes as h cross root of l into l+1 right. So, actually you get the Eigen value of l square as h cross square times l into l+1. So, the order of magnitude value of the angular momentum will be given by the square root which is h cross times l into l+1.

And now you can strike out the h cross on both sides and for large values of l, l+1 will be very nearly equal to l. And you have got you are looking at a square root of l square which is l itself.  So, the order of magnitude estimate for l max is that it will be of the order of a into k. So, depending on the finite range a how large it is and depending on k and what determines k it is the incident energy which is h cross square k square by 2 m right.

So, depending on the energy of the incident beam and depending on the range of the potential there is a certain maximum value beyond which you really do not have to consider the scattering. Because the classical particle will simply go past the target area without interacting with it okay. So, this is the idea behind having a maximum  partial wave contribution.

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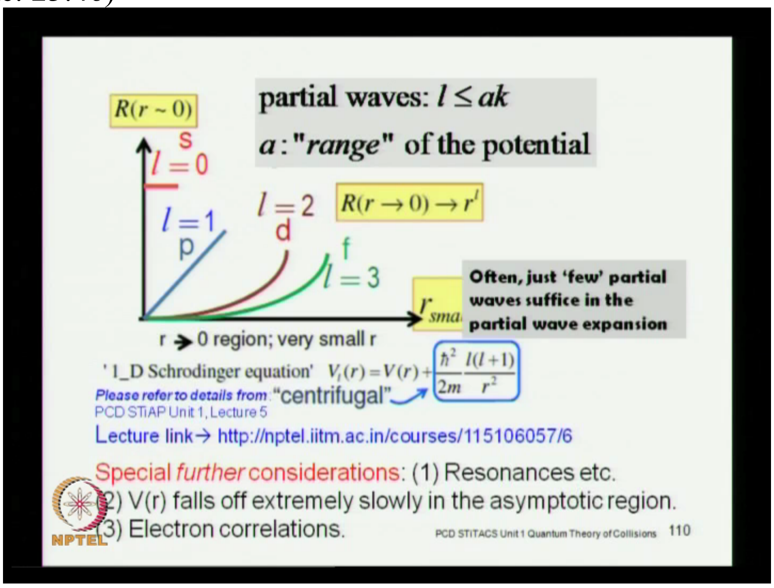


And you have to consider only those values of l which are less than or equal to a times k. Now this value can be pretty large it can be 100, it can be 200, it can be a 1000 but not infinity okay. For 1 over r has to be considered in a completely different way. So, good, good point and like I said that this entire discussion of the partial wave analysis in which we have only an energy dependent phase shift, a k dependent phase shift.

Is, we already discussed it in an our, in some of our earlier classes that this is valid for those potentials which fall faster than 1 over r okay. The Coulomb potential has to be dealt with separately okay. You have a logarithmic phase shift in that case. So, that is a separate issue but for most of the potentials which fall faster than 1 over r this method works and you have some idea of a range.

It is not very strict and the way to do it is very often what here is do is, to do this calculation up to a certain number of partial waves. They consider like 100 then add another 10, another 20 and then at some point it really converges and you really do not have to add any further because if the additional contribution from the other partial waves from the higher partial waves is not of importance there is no point in including it in the partial wave analysis.

Now this is completely consistent with the picture we have because we know that the radial function goes is r to the power l as r tends to 0. So, closer to the target okay, the s waves always reach closer to the target. The p waves also reach but at the target they already go to 0 right and higher the value of l the faster does the radial function go to 0.

So, the partial wave really does not get into the core and which is completely consistent with the fact that it is not get involved in the sketching process because to be able to get scattered it has to interact with the target and that is going to be possible if it gets into the core of the target. And that happens most for l = 0 and least for higher values of l as l increases.

This, the chance of the radial wave entering the code decreases in fact this already becomes parabolic for l square for l = 2 for the d ways. For f waves you know they go to 0 even faster. And this is because of this centrifugal term in the radial Schrodinger equation right. So, we have discussed some of these details in the previous course and you can see this at this link but I will not repeat those arguments over here.

So, typically just a few partial waves are sufficient to include in the partial wave analysis. There of course are some special considerations may be have to make exceptions for those situations where we have resonances. You may have a situation in which Vr falls off extremely slowly in the asymptotic region okay.

So, there may be some peculiar physical potential for which we do not use this type of consideration. But for most of the situations you are able to cut off the partial wave expansion at a certain maximum limit. So, that you do not have to consider infinite terms. Besides this entire thing discussion is within the domain of the single electron approximation.

There are these electron correlations and many body facts which we have not taken into account. So, all these will add certain exceptional additions to our consideration and they will have to be analyzed separately.

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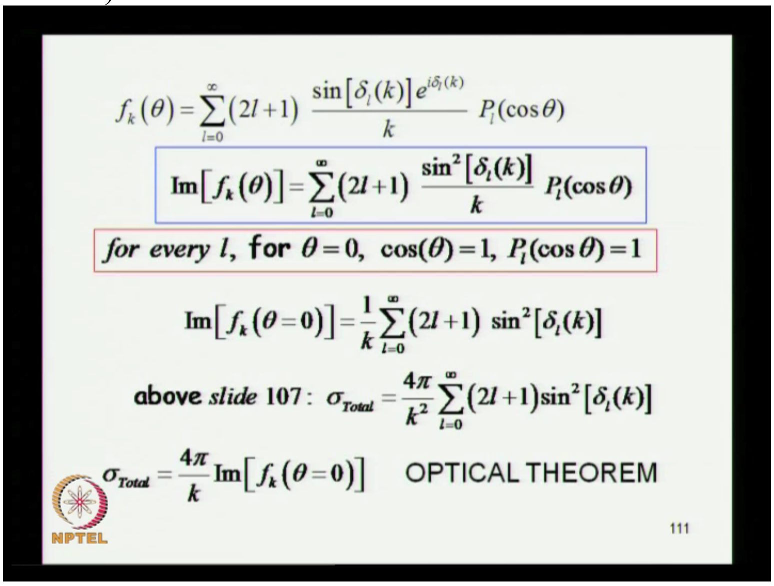


So, let us go back to the expression for the sketching amplitude. Now you have got a complex number here which is e to the i delta okay, which is cos delta + i sine delta. So, if you look at the imaginary part of this scattering amplitude it is sine delta sine delta multiplied by this sine delta gives you the sine square delta right. This is the imaginary part of the scattering amplitude.

And if you look at forward scattering for theta = 0, cos theta = 1, Pl cos theta = 1, for every value of l. So, for forward scattering what do you get? For forward scattering you get the imaginary part of the scattering amplitude for theta =0, which is 1 over k, this 1 over k is coming from here, summation over l going from 0 through infinity 2l + 1 comes here. And then you get a sine square delta term.

But then we have seen earlier just a few slides earlier that the total cross section is given by a similar expansion which is 4pi over k square times this summation. If you look at these two summations you really find that they are the same summations right. Essentially the same summation which means that there is a relation between the sigma total and this part and if you just combine these two terms, you get the optical theorem once again okay.

You recover the optical theorem as a very general theorem and this is not dependent on any approximations like neglecting 1 over r square terms or anything like that means. Earlier we had used equation of continuity to discuss and obtain the optical theorem. This time there is a different route but essentially to the same result.

That the total scattering cross section is given by 4pi by k times the imaginary part of the forward scattering amplitude. We are now going to discuss a more general form of this theorem in which we will also exploit the properties of the scattering operator which we will first have to define.

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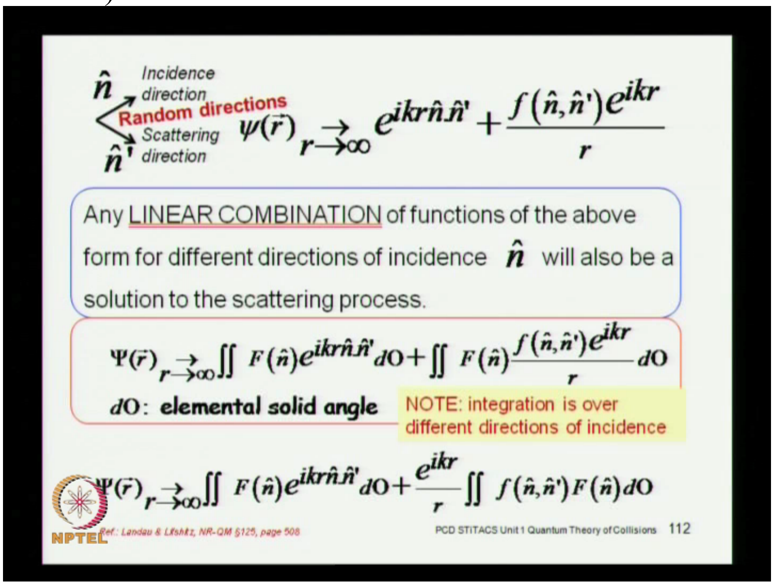


So, to consider that let us first consider scattering in which there is the incident beam is incident in a particular direction n. This carrot, this hat symbol presents a unit vector it is just a direction. So, let the incident direction be indicated by this n carrot. And the scattered direction as n prime these are just two directions in space.

Now typically the incident direction could be anything. I can have a target here and I can have an incident beam coming from here, I can have an incident beam coming from here, I can have another incident beam coming from here right. So, in general that direction of incidents in principle could be anything.

And you can think of random directions and the solution for a given direction of incidence is has got this form up apart from normalization. So, we will not worry about the normalization. So, you have got the e to the ikr, the cosine of the angle between the two directions the incident directions and the scattered direction.

So, that is the incident plane wave with this term and then you have got an outgoing spherical wave along with the scattering amplitude. Now this is the general form of the solution for a given direction of incidence. But any linear superposition of functions of this form for different directions of incidents will also be a solution okay.

This is not a unique solution so if you just superpose solutions of this kind for different directions of incidents that will also be a solution. So, the general solution for the asymptotic region will be a summation for different values of n. But the direction of incidents can change continuously. So, you really need to consider integration and you can change angles with respect to both azimuthal angle as well as the polar angle right.

So, now with reference to a reference direction given by the scattered beam, scattered particles the scattering is taking place in the direction of n prime right. So, with reference to n prime the direction of incidence n is changing and the integration is now over different directions of incidence.

Which is why this solid angle d omega I have written as dO, this is the solid angle in which the variations are coming from different directions of incidents not the different directions of scattering okay. So, this is in a double integration this is an elemental solid angle d omega so it has got a similar expression like sine theta d theta d Phi.

But now the reference direction is not the direction of incidence but the direction of scattering so it is a different geometry right. So, this is also a solution to the sketching problem. This is a mathematical construct it does not represent a physical situation okay. In a physical experiment which you carry out in a laboratory you have got the target placed okay. You got a projectile beam okay.

So what an electron gun or you know whatever is your source of the projectiles and this is the direction of incidence. So, this is a mathematical construct which I am using to demonstrate some very powerful properties of the S matrix. So, this is the general solution for different directions of incidence, mathematically it is strictly correct. And in the form which I have written at the bottom, I have extracted this e to the ik r by r outside this integral.

And inside the integral I have got this f nn prime and this fn which is like an amplitude corresponding to a different particular direction of incidence right. But mind you the relative amplitudes between the incident beam and the scattered beam are completely determined by the coefficients over here okay. The 1 over r takes care of the fact that the sphere area expands as our square right.

And the angular dependence is completely taken care of by the scattering amplitude. So, this is only a weight factor which keeps track of the different directions of incidence. It is not contributing to the relative weight between the incident beam and the scattered beam okay. That is completely determined by this f over r term right. So, this is your expression for the general solution for different directions of incidents.

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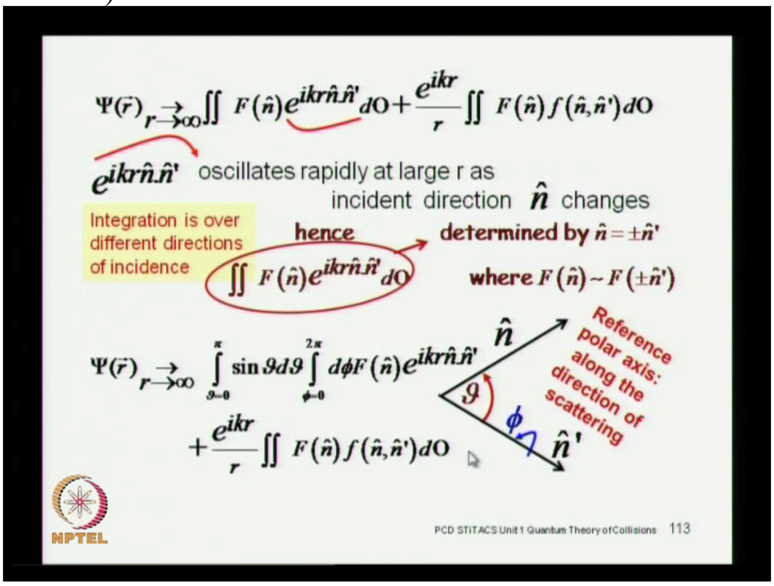


Let us look at this term and notice that at large values of r for different directions of incidence. The angles will change okay and the cos theta will change and there will be an oscillatory destruction of this term. And the only terms which are going to survive are those for which this e to the ikr n dot n prime has got an extremum.

So, that cos theta will have to be either +1 or -1 okay. Those are the two terms which will make a meaningful contribution because this integration is over different directions of incidence and this value of the first integral is completely determined by either the forward direction or the backward direction.

The direction being specified with respect to the direction of scattering which is n prime, so n = + n prime or n = - n prime are the two directions of importance of our first integral is concerned. And for these two directions the corresponding F function this uppercase F function will be either, F of +n prime or F of -n prime appropriately right. So, the reference direction in our case which is being referred to as a polar axis is the direction of scattering.

And this is a different theta and a different Phi then I had used earlier okay. So the polar angles are measured with respect to this direction. And the azimuthal angles are measured with respect to this direction. So, now you have to carry out this integration with respect to theta and Phi the different directions of incidence okay.

So, this is the solid angle sine theta d theta d Phi theta going from 0 to pi and Phi going from 0 to 2pi. And then from the second integral you have got a similar expression right.
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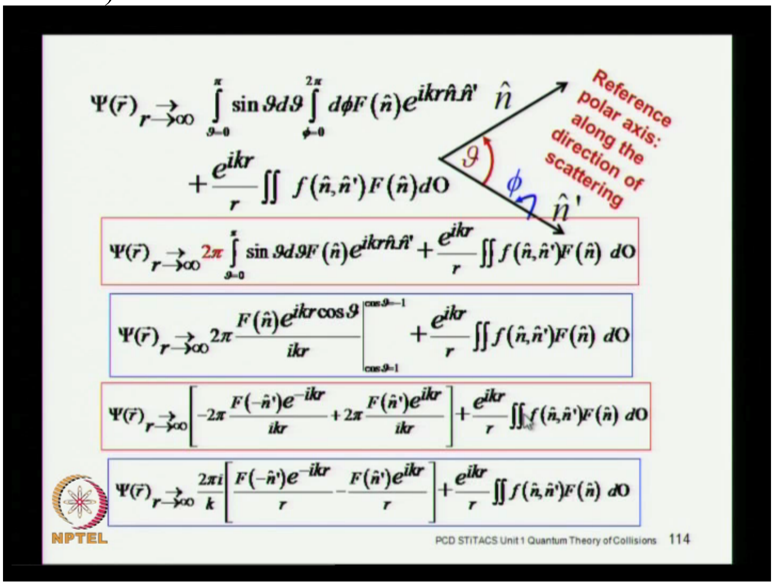


Now this is the expression that I brought to the top of this slide over here. And if you now carry out the integration over this azimuthal angle Phi you get a factor of 2pi then you get integration over theta, integral sine theta d theta then you have got this f function then you got e to the ikr cosine of the angle between the two directions n dot n prime.

And from the second term you have e to the ikr by r and then this double integral which is integration over the two angles polar angle and the azimuthal angle right. Now let us look at the first integral here, this is integral over theta and this year the function is cosine theta. So, you can transfer the integration variable from theta to cos theta. So, you will get a - sine theta d theta right.

And you all you have to do is to take the difference in the value of f e to the ik r by ikr at the two values the upper limit will be cosine theta = -1 because there is a -sine theta d theta so this limit will go to the top cos theta = -1. And this will be cos theta = 1, so you have to take the difference of the value of this function at these two limits right from the first integral, the second integral is written as it is, is it clear everybody very good.

So, let us take this difference put cos theta = -1 and subtract from it, the value of this term for cosine theta = +1. So, for cos theta = -1, you have e to the ikr and you have a minus sign over here. So, you have this F of n will be F of -n prime right. And then you have got 1 over ikr + 2pi times the other term which comes at cos theta = +1.

So, you got e to the ikr over ikr and here this F function will have an argument which is n prime because for cos theta = 1 theta = 0 and n will be equal to n prime right. So, these are the two terms coming from the first integral the second integral is written as it is okay. So, these are the two terms and I take this 1 over i to the top that will give you a 2pi i.

But then you have to take care of the sign because when i goes to the top it picks up a minus sign right. So, you have got a 2pi over k F - n prime e to the - ikr by r, the 1 over k is outside and this is Fn prime, the 2pi is also outside this i has already been taken care of and you got Fn prime e to the ikr over r and the second term is written as it is okay.

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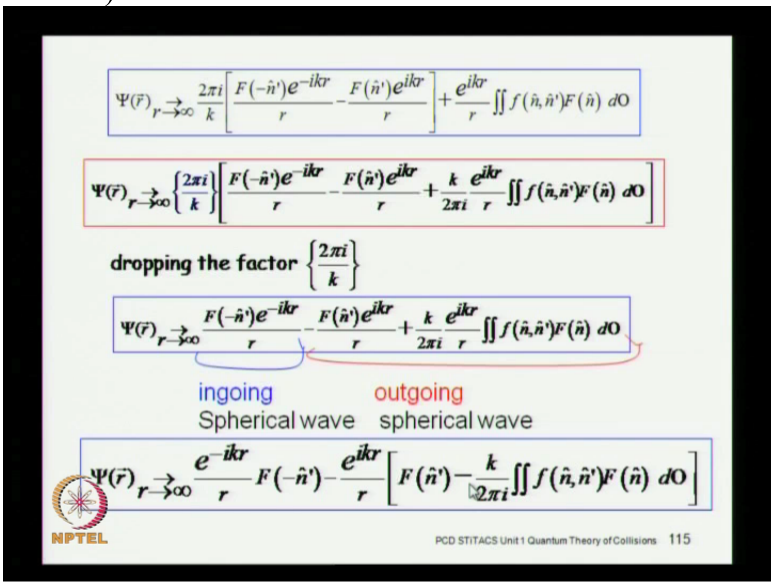


So, we bring it to the top of this slide here this is the previous expression. Now notice that I have now taken 2pi by k common not just to this term but also to this term and to compensate for that I get a k over 2pi over here okay. So, I have combined these two terms with the third term which is this double integral and to compensate for this 2pi over k which is in this common beautiful bracket.

I get a k over 2pi i to take care of it and this 2pi over k is a common term which can always be absorbed in the overall normalization so, I will drop it for a simplicity. And the remaining terms is what is inside this rectangular bracket which I have written over here. Now this is the ingoing wave and this is the outgoing wave right.

This is e to the ikr over r, this also e to the ikr over r and these two terms contribute to the outgoing spherical wave and this contributes to the ingoing spherical wave. So, the outgoing spherical wave is e to the ikr over r and these two terms I combine. So, I have got a minus sign over here.

And what is the other factor which multiplies e to the ikr over r is this is this Fn prime times this k over 2pi i times this double integral over the solid angle okay. So, let us analyze this expression further,

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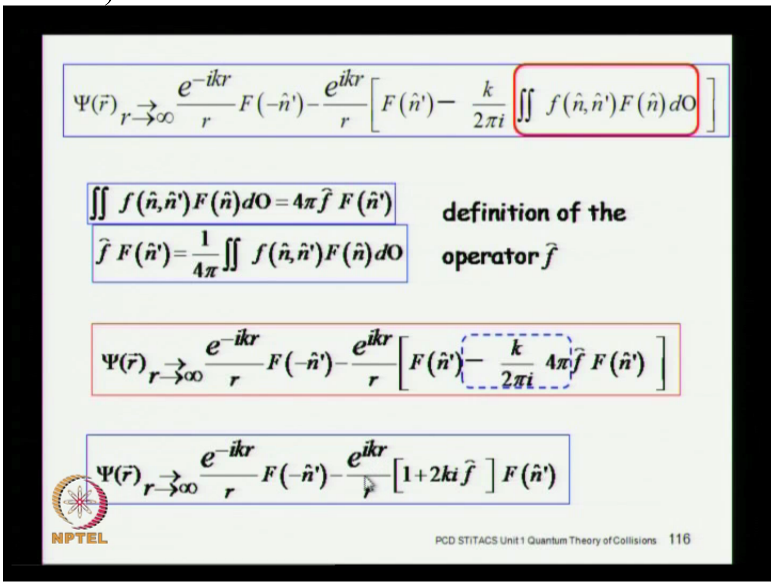


here we have it. Now look at this term this is the double integral over the two angles azimuthal angle and the polar angle defined with reference to the direction of scattering right. The direction of scattering is n prime the direction of incidences n the integration is over the incident direction which is represented by unprimed variables okay.

The primed variable is a fixed one which is the direction of scattering that is the reference direction. So, let me now define an operator written as f cap okay. This is not the carrot V shaped hat it is an arc shaped at slightly different shape just to remind us that this is not a unit vector or anything like that.

It is a new operator which is being introduced now and it is being introduced through this definition that this integral in this double integral is equal to 4pi times this f operator operating on this function f. What is this function of it is a function of a certain direction in space okay. It does not contribute other amplitudes and so on to the scattered wave length scattered particle right. But it only depends on a particular direction.

So, this is the definition of the operator f or you can write this equivalently as f operating on F as 1 over 4pi times this double integral. This is the definition of the operator f. Now using this definition we can write this expression, the first terms is the same e to the -ikr by r and then this function F of -n prime.

This is the spherical outgoing wave e to the -ikr by r. You got this function here and the second term is k over 2pi i times 4pi times this according to this definition of the operator f okay. Now if you look at these two terms here this you can simplify first you have got a 4pi over 2pi so that will give you a factor of 2.

So, you can write this as the first term, the second term is e to the ikr over r and combining these two terms you can write this as if you have got an another operator in this rectangular bracket which is some of the identity plus the 2ki times the operator f operating on this function of direction right.
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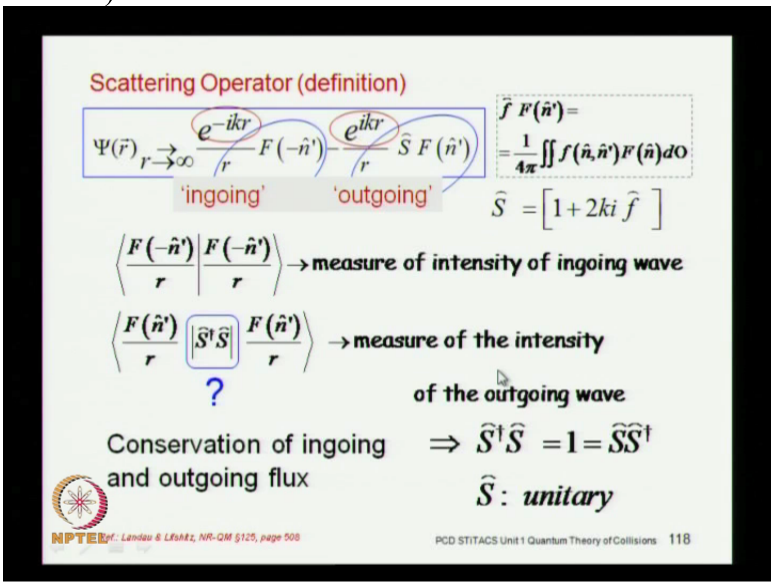


So, this is what we have got and in this the new operator which is defined is this f which is defined through this relation. What we do now is to take this operator 1 + 2ki times f and this is our definition of the scattering operator. This was first introduced by Heisenberg in 1943 in his formulation in his reformulation of quantum mechanics in terms of the scattering operator.

And in terms of the S operator this is called as the scattering operator this is now the definition of the scattering operator which is defined in terms of the operator f and the definition of the operator f is here. So, this is the definition of the scattering operator and in terms of this definition the general form of the solution is e to the -ikr over r F -n prime coming from here -e to the ikr over r.

This is the scattering operator S operating on the function f right. Now let us see what this leads us to, notice that this is the incoming part or in going part, this is the outgoing part right. What are they weighed by, they are weighed by these factors in the blue loops this by F -n prime by r and this by SF over r right. These are the corresponding weight factors of the ingoing flux and the outgoing flux.

Now the measure of intensity of the ingoing flux will be given by this inner product F-n prime over r right. This is the norm corresponding to this part this will be a measure of the intensity of the ingoing wave. What is the measure of the intensity of the outgoing wave; you have got a similar inner product, scalar product composed from this term.

What is that? You have got SF over r and this is S dagger f over r right. So, this is a measure of the intensity of the outgoing wave. Now what goes in has to get out this conservation of flux you are not creating particles, you are not destroying particles right, you are only scattering them.

So, the measure of the intensity of the ingoing wave and the measure of the intensity of the outgoing wave must be the same. What does it tell us this is essentially the conservation of the ingoing and outgoing flux; what does it tell us about this operator? Yeah (Question not audible) it must be unitary right.

So, we conclude that the operator S must be a unitary operator and this is just a statement of the conservation of flux. So, the Unitarity of the scattering operator is connected with the conservation of the flux

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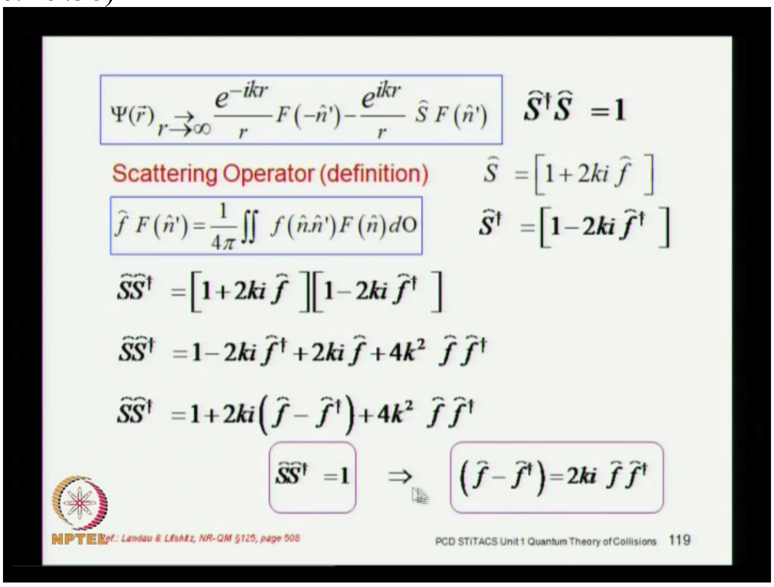


And we use this property of the Unitarity of the S matrix. And how did we define the S operator this operator is defined in terms of the f operator as 1 + 2i k times f right. This is the definition of the scattering operator okay. So, given S we know what is dagger is, so let us construct SS dagger which is just the multiplication of these two operators.

Multiply them out term by term. So, you get 1 - 2ki f dagger + 2ki f + 4k square ff dagger right. And you combine these two terms 2ki is common to both, so you get f - f dagger here

and notice that SS dagger = 1. So, you must get this term and this term must cancel each other right. Which means that f - f dagger must be equal to 2ki times ff dagger.
So, this is an identity which is an automatic result of the Unitarity of the scattering operator, so we will now use this identity.
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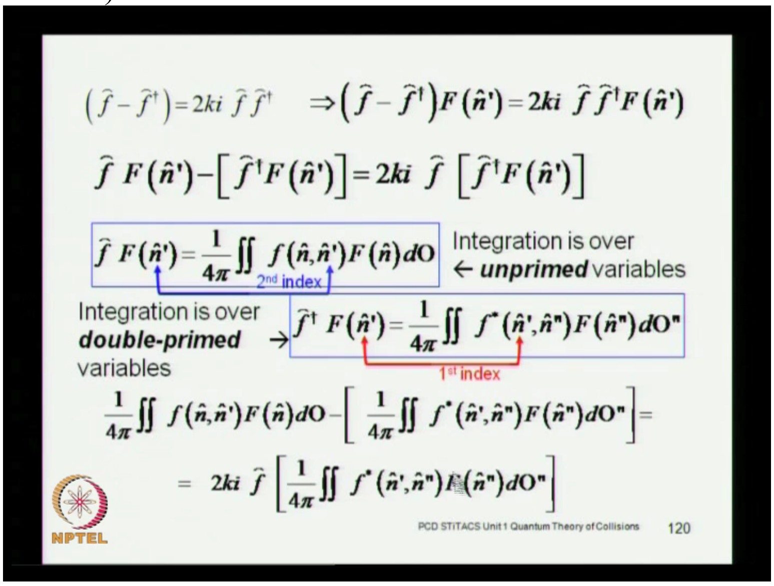


So, we consider this identity which means that if this identity is to operate on an arbitrary function of this direction n prime you have this result. And you have two terms on the left hand side right. On the right hand side you have got 2 ki i times, 2ki times f operating on f dagger of this. So, you carry out this operation first, how do you do that? You know what f does to F right.

So, you can figure out what f dagger will do to F okay because this is the adjoint operator. So, what it will do is you have to keep track because when you do the adjoint. You have to take into consideration the complex conjugation and also the transposition right. So, here this n prime is the second index as we get from the definition right and the integration is over the unprimed variable which is n.

So, over here we can define f dagger F in a similar fashion but now you have got the complex conjugation f star and the integration is over the double prime variable which is the dummy you index. The index which is not dummy is the direction indicated by the function on which you are carrying out the operation. So, f dagger operates on F of n prime, so n prime is the argument of this F.

So, this is not a dummy, so this will be the first index, in this case this was the second index right. So, here the integration is over the dummy double primed variable in the first the integration is over the unprimed dummy label. And you know put f operating on F by this double integration. The second term is - f dagger operating on this which is coming from here this is f dagger operating on this.

And then on the right hand side you have got f operating on f dagger operating on F. So, you have got this 1 over 4pi times this okay. You have to do this carefully it is very easy to make a careless mistake. So, notice that 1 over 4pi is common to all the three terms. So, you can cancel them right, you can leave them behind when you carry this relation to the top of the next slide.

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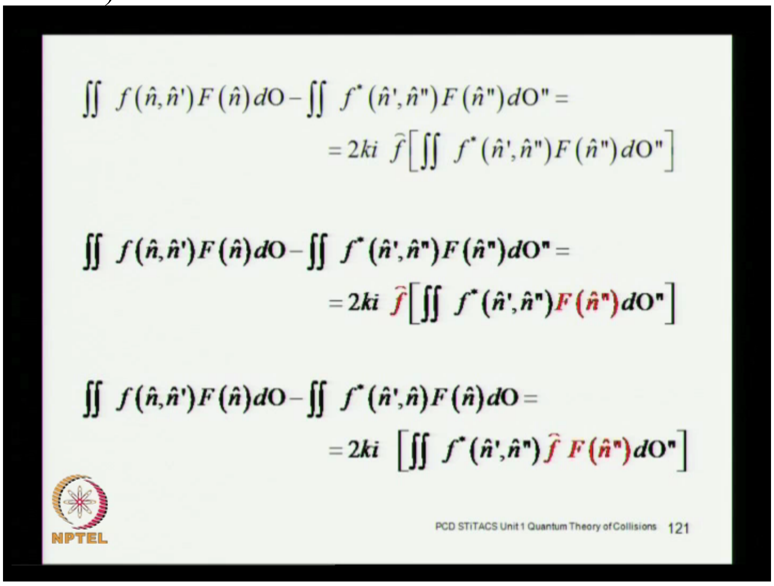


So I have left over there 1 over 4pi factor the rest of the terms are here. And now notice that on the right hand side you still have to carry out one operation which is this operator f operating on F this is this operates only on the function F this is just the scattering amplitude right.

So, f operates on this direction function F of n double prime, so this operator f the only part of the operand on the right side which is of importance for our consideration is this function F. So, f operating on F is what we want to find out but now the argument is double prime not the single prime, so you have to be careful in choosing the dummy index. So, this is the function to be dealt with this operator f operating on F.

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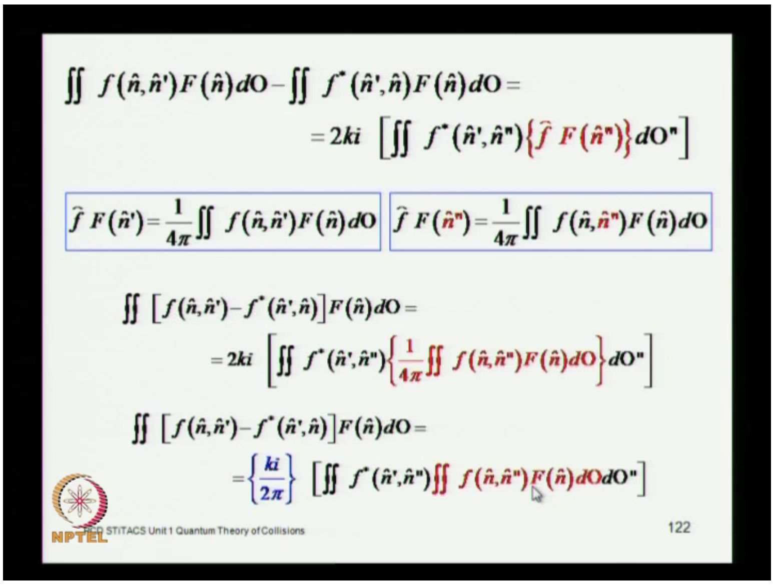


So, let us work on this term alone rest of the terms are already taken care of and this we you get from the definition of the operator f itself. But we had defined it with reference to and scatter direction n prime. Now we want to define it where we want to use it for a scatter direction in double prime okay. So, with reference to the double primed direction you need a different dummy index which I have used as the unprimed index okay right.

Because there is no unprimed index over here and this term, so there is no hassle okay. So, now let us write all the terms, so you get the first term is here from this two differences. Both our integrations over the same solid angle the same functions. So, you can take the common factor in the two integrands which is f - f star multiplied by this common factor uppercase F.

And then on the right hand side you have got these two integrals right. And now on the right hand side you have got 2ki over 4pi, so that gives me ki over 2pi rest of the terms I have retained as they are which we will simplify in the next step okay. Here I only take care of the 2ki over 4pi.

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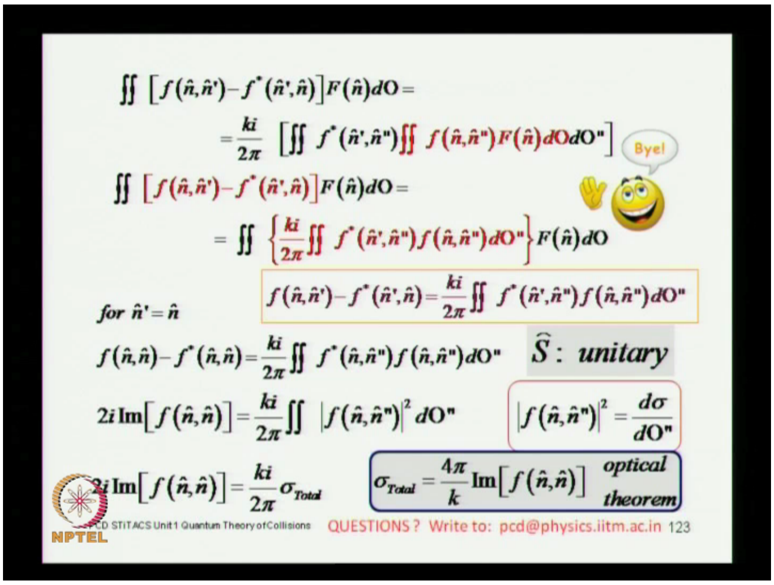


So, that gives me ki over 2 i on this side and here look at this integral here there is an integration or unprimed variables and integration over primed variables. What are the integrands, integrands contain n prime, n double prime n and n n double prime. So, what is going to matter with reference to the integration of what the double prime variables are only these two terms okay? F is not a function of the double prime.

So F can be taken outside and the rest of the terms which are important with reference to the integration over double prime the integrals can be combined together. And now look at these two integrals on the left hand side as well as the right hand side you have got integrations over the same variables.

These are definite integrals and by comparing the integrands you have the result that f - f star = ki over 2pi times f star f integrated over the double primed variables. Keep track of the positions of the arguments. The directions n prime and n double prime this was the first index here which went with the complex conjugation and here the dummy index is the second index here okay.

So, you have to keep track of which is the first index and which is the second index and which is the dummy variable okay so keep track of that. So, this is what we get and if you look at this result and specialized it for the case that n prime = n. So, this is valid for every value of n prime right.

So, if you look at it for the particular value of n prime namely the value n prime n, then on the left hand side you get f n n -f star n n = ki over 2pi. And now this n prime has been set = n the second index here is n double prime the first index here is already N and the second index is the dummy variable in double prime right.

What do you have on the left-hand side you have got a complex number from which you are subtracting its complex conjugate. So, you get twice 2i times the imaginary part of that complex number which is 2i times a imaginary part of this scattering amplitude which you can already see is the forward scattering amplitude right on.

The right hand side for n n prime = n you have put this n prime equal to n, so you got f star n n double prime f n n double prime, so that will give you the modular square of this amplitude right. And what is this square of the modulus of the scattering amplitude, it is the differential cross section d sigma by d omega right. And it is this d sigma by d omega which you are integrating over the all the angles okay.

So, you get essentially the total cross section out of it so that is what you get the 2i times imaginary part of the forward scattering amplitude is equal to ki over 2pi times the total cross section. And you can see that this is already the Optical theorem and we have connected it with the Unitarity of the scattering operator.

It is connected with the conservation of flux and I will be happy to take any questions at this point but essentially the optical theorem is a very powerful theorem. And we have had different approaches to the optical theorem from different angles. We have considered the probability current density vector in one of our earlier classes then we considered the partial wave expansions a little earlier in today's class.

And now we have introduced the scattering operator we have established the fact that the scattering operator must be a unitary operator the way it has been defined by Heisenberg right. And this is an essentially unitary operator connected with the conservation of flux and this is at the heart of the optical theorem.

Be happy to take any question(Question time:1:00:41) by comparing the ingoing and outgoing flux and yes getting this thing, so actually what will be the Psi star Psi, so Psi star Psi will contain some another some interference kind of density. Yeah we have considered those when we did the current density vector analysis. In fact it is the consideration of the interference term which led us to the optical theorem at this point I will stop here for today.