Select/Special Topics in 'Theory of Atomic Collisions and Spectroscopy'
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Lecture 06
Differential Scattering Cross Section, Partial Wave Analysis

Greetings, we will today complete the proof that the relation d sigma by d omega is the square of the modulus of the scattering amplitude is valid also when the incident beam of particles is described by a wave packet. Which may have a little bit of you know dispersion. So, that it is not strictly mono energetic and there may be a little bit of energy spread and then we will get back to our discussion on partial wave analysis.

Which will be the primary subject of this unit and there is a lot of discussion that will follow using the partial wave technique in this unit, in unit 1. So, I will probably take a somewhat more number of classes for unit 1, then I had originally planned because the partial wave analysis is a fairly large topic. So, will we, will see how it goes. But today we will complete this proof and then get back to the discussion and partial wave analysis.
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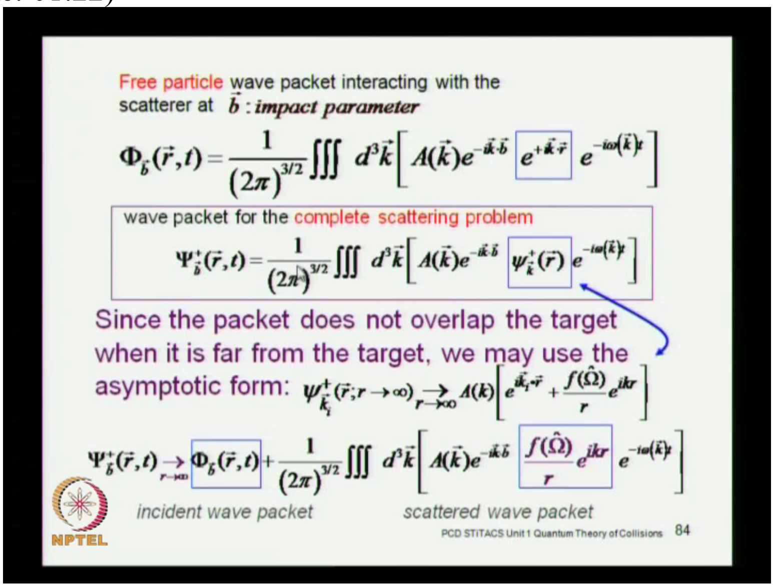

Now we had described the wave packet corresponding to free particles in the incident beam and then we reconcile with the fact that the incident beam may not confront the target head on. But there may be a little bit of displacement in terms of what we call is the impact parameter. So, that the centers are shifted a little bit, center of the wave packet may be little bit shifted and that was described by this impact parameter.
Now notice that this impact parameter is if the incident beam is coming like this in the target is here the impact parameter is in a plane which is perpendicular to the direction of

propagation okay. The vector b is completely in this plane it is orthogonal to the direction of incidence so just remember that.

And with reference to that vector b we write the incident wave packet with the subscript b and this e to the ik dot r is then corrected to e to the ik dot r -b which is how you get this e to the minus ik dot b term over here. So, this is the free particle wave packet and the solution for the complete problem inclusive of scattering.

When you have a potential which scatters the incident particle beam is given by the replacement of this free particle term e to the ik dot r by the appropriate complete solution to the problem indicated by the superscript plus corresponding to the outgoing wave boundary conditions. So, it will include the incoming part as well as the outgoing wave part right that is the total solution to the Schrodinger equation along with the scattering potential.

So, this is the complete scattering problem solution and because the wave packet is will it will not be in the same region as the target itself when it gets to the detector. We use the asymptotic form which is quite a property to be used over here and we know this asymptotic form for an incident unit vector, incident momentum vector ki to be given by this energy dependent normalization.

And then there is an incident mono energetic wave over here corresponding to that particular vector ki and then there is the scattered part which includes the scattering amplitude and as an outgoing spherical wave e to the ik r scaled by the 1 over r right. So, this is the scattering solution this will go over here and then it will become a part of this integrand in the complete solution to the scattering problem.

So in terms of the wave packet description you have got an incident wave packet corresponding to the impact parameter b which is what we have written in the first row over here. So, this is the incident wave packet and the scattered wave is given by this in which the outgoing scattered.
Outgoing wave boundary condition solution is includes the scattering amplitude and the spherical outgoing wave e to the ik r scaled by one over r. So, this is your scattered wave packet this is the incident wave packet
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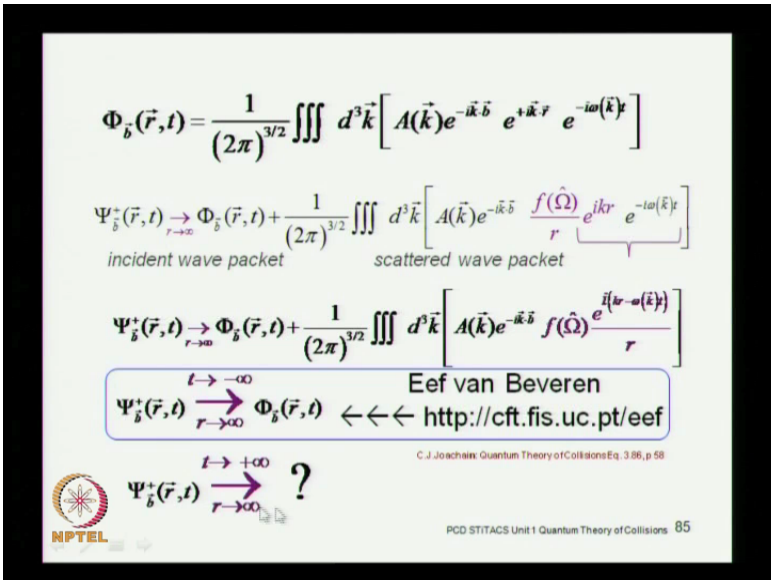

Now let us look at some of these terms. You combine these two together to write this spherical outgoing wave. So, this shows the explicit time dependence and how surface of constant phase is a spherical wave which is radially going outward. So, this these two terms have been combined over here and if you look at the form as t tends to minus infinity.

That is much before scattering took place which is when you would have only the incident wave packet which is Phi b r of t. Now this can be shown quite rigorously using mathematics and I will refer you to this proof in Beveran's article which you can refer to. But essentially you can see that as t tends to minus infinity you will have only the incident wave packet corresponding to the impact parameter b.

But then our interest is in t going to plus infinity that is when you will detect the solutions to the scattering problem okay. That is what the detective will record and then you will get; you will seek information about the scattering potential from what you observe in the detector. So, this is the fundamental quantity of interest.

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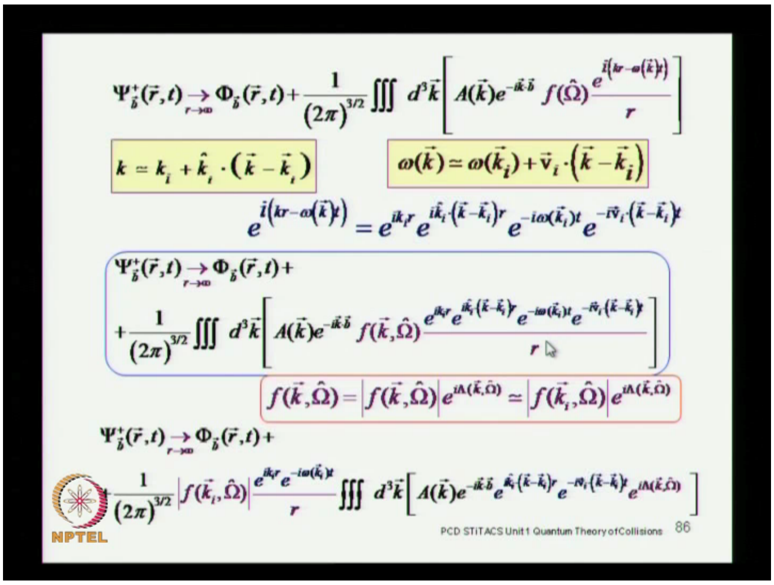

So, let us have a look at these terms and this we know is given by the combination of the incident wave packet and the scattered wave packet. Now k is not strictly equal to ki a single momentum as such. But it could change in the vicinity of that but not very much because it is a nearly mono energetic beam. So, we take the first order correction to this which is ki dot k - ki right. So, that will be the value that k will have.

Likewise omega which depends on k, we have already seen that if you expand it around an initial momentum. You took another the first order correction to that and we have seen that it turns out to be this you get the gradient of omega but we have seen how the gradient of omega is evaluated and it turns out to be this. We have done this in the previous class.

So, using these two terms we write this phase factor this is e to the ik r - omega t. So, from this kr you get two terms one coming from ki which is this. The other coming from this term which is ki dot k - ki times r. So, that is what takes care of e to the ik r then you got e to the - i omega t. But omega consists of two terms one for omega ki which is here and the other from the gradient of omega which is over here. So, those are the two terms right.

So, we will now write all of these terms explicitly. So, instead of this factor we will have this expression here. So, you have got the incident wave packet in the complete solution for the impact parameter b and the scattered part in which you have written this factor in terms of these different factors which multiply each other to give you the complete phase.

Now this is the complex scattering amplitude you write this complex number in the form Rho e to the i theta. So, this is the amplitude and this is the phase, this is e to the i lambda, this is an upper case lambda. And this is how you write the scattering amplitude and this will not change very much for small way variations in the incident direction.

So this scattering amplitude for the wave vector k is very nearly equal to the scattering amplitude for the wave vector ki which is a particular value of the incident momentum about which we are carrying out the expansions and then there is a phase which may however change because the phase is very sensitive to directions.

So, now from this the integration is over the vector k in three dimensions in the momentum space. So, whatever factor you find in the integrand which depends on a particular value of k which is ki which is the value about which you are carrying out all the expansions. All of those factors will be constants inside the integration right and they can be pulled out.

So, this sketching amplitude has been pulled out over here. Likewise these two phases e to the ik ir and this is the value of the circular frequency omega at the value ki. So this is also pulled out of the integration and all the other terms are retained inside okay, 1 over r of course is independent of k, so that is also taken out.

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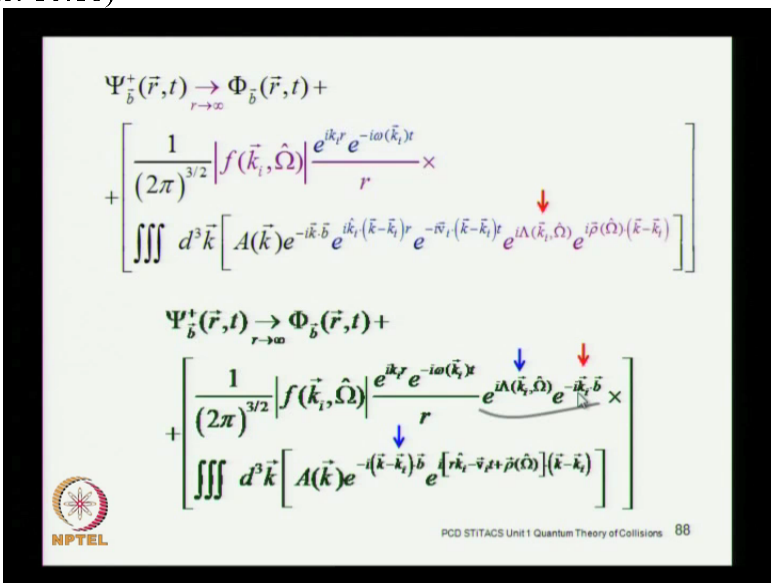

So, we bring this to the top of this slide over here and again we now look at the momentum dependence of the phase lambda, this is the phase of the complex scattering amplitude. So, again you can expand this angle about the value corresponding to the particular value ki. And then again you have the first order approximation and you will have the gradient of lambda dot its scalar product with the difference of the momentum of k and ki.

And this gradient is what we call as Rho at a particular angle omega. So, with this definition of Rho, which is given by the gradient of lambda, you now have this lambda k to be given as lambda ki plus this Rho and there are these two terms which will come here. Out of which the one corresponding to ki will be a constant under the integration and that can be taken out okay.

So, you have these two terms one is here, this is the lambda at ki and this is the Rho dot k - k i dot, all the other terms are pretty much the same as they were in the previous expression. So, this is what we have got we have got these two terms now one is lambda at ki and the other is a rate at which lambda changes with k that is the gradient of lambda dotted with k minus ki. All the other terms are essentially the same.

And since this term depends only on ki this e to the i lambda at ki can be pulled outside the integration sign okay. So, pull it out and this has now come outside the integration you have got the first factor which multiplies this integration in the momentum space. So, this factor is now taken outside the integration. What is also taken out is this e to the - ik i dot b, first of all we agree that it can in fact be taken out.

Because it depends only on ki and a constant b which is the impact parameter so it has no dependence of the momentum vector over which integration is pre carried out. But then this factor did not exist in the integrand. So, you compensate for it by having this; you have e to the -ik r dot b, so inside the integration you add an e to the + i ki dot b over here okay.

You see that the other term is of course -ik dot b which was there in the integrand already. So, this is the extra term that you are pulled out and you have compensated for it over here. So, that your integrand is well balanced, it is continues to be what it was as you manipulate these terms.

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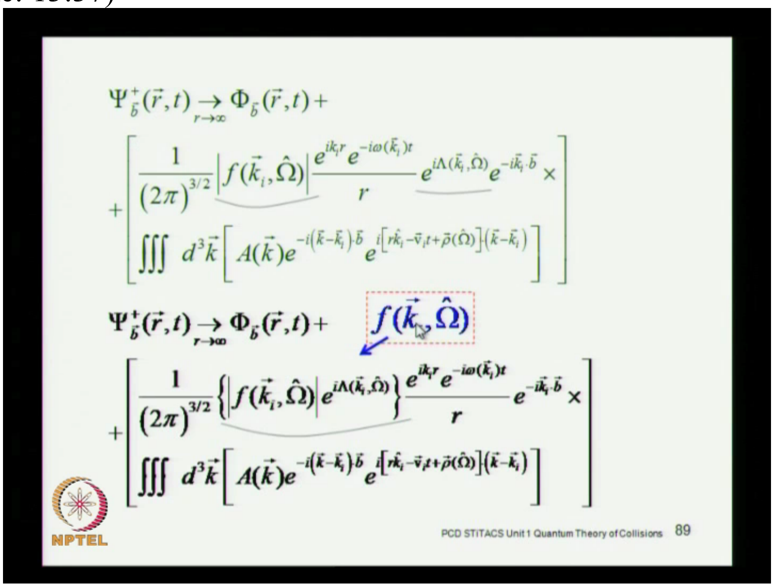

So, now you have got those terms which depend on ki which are factored out of the integration and inside the integration you have got a number of terms. Now look at this one this is the magnitude of the amplitude this is the phase at that particular direction of incidence. So, these two can be combined and together they give you the complex amplitude at the vector ki okay.

So, now that you pull this out this factor had already been brought out and together you can combine these two terms to write this complex amplitude corresponding to the incident momentum vector ki, corresponding to scattering amplitude in the direction omega. Omega is a particular direction in the space right.

So, that is the direction in which scattering is taking place and this is the measure of the probability amplitude further for scattering in that particular direction okay.

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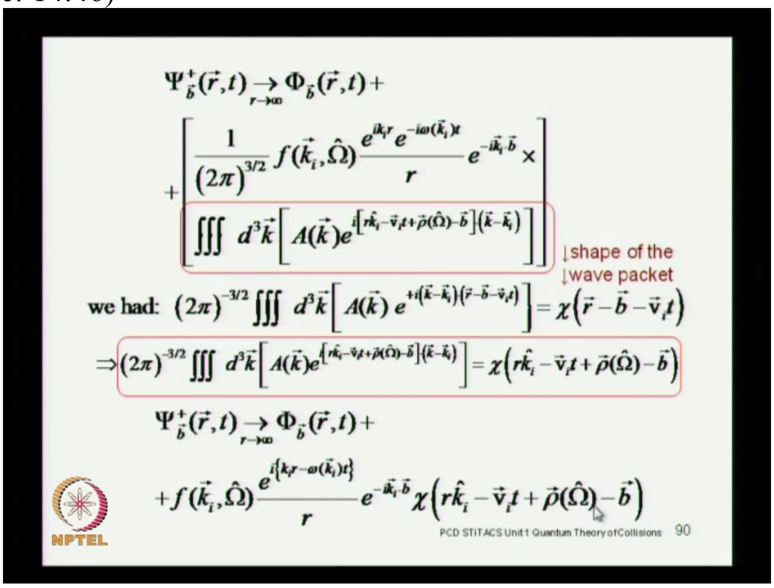

So, this is the complex scattering amplitude so the modulus and the phase have both gone into this. Rest of the terms are the same and if you look at this term here, the integration now have you met this integral earlier. We have in fact dealt with this earlier already do you recognize it, is this not the shape function okay.

This is the same type of integration means together with this 1 over 2pi to the 3 half, we had defined with this 1 over 2 pi to the - 3 half integration in the momentum space of this energy dependent normalization and e to the i theta where theta was a certain phase which was given in terms of the scalar product of k - ki and a certain distance vector.

This was our definition of the shape function and the distance vector had this arguments r and b and also vit, so these were the arguments, so this is pretty much the shape function with the difference that the argument of this distance vector is somewhat different but it is pretty much the same type of integration right.

In other words we can rewrite this what you have in this red loop this expression which you read now recognized to be the shape function this is the same shape function except for the fact that its distance vector argument is not r - b –vit, but it is given by these 1, 2, 3 and 4 terms okay. So, those 4 terms come over here 1, 2, 3 and 4 all of those four terms.

So, essentially you have the shape function it is exactly the same integral and you have a shape function and you can now write this complete solution to the scattering problem in terms of this incident free particle wave packet arriving in at an impact parameter b plus a scattered outgoing part in which you have got a complex scattering amplitude here.

Then you have this phase factor here e to the ik ir - omega ki t. Notice that there is only one momentum in these two terms which is ki. Then you have got a term in e to the -ik i dot b, which comes here and then you have got this integration in the momentum space which is the shape function with this argument.

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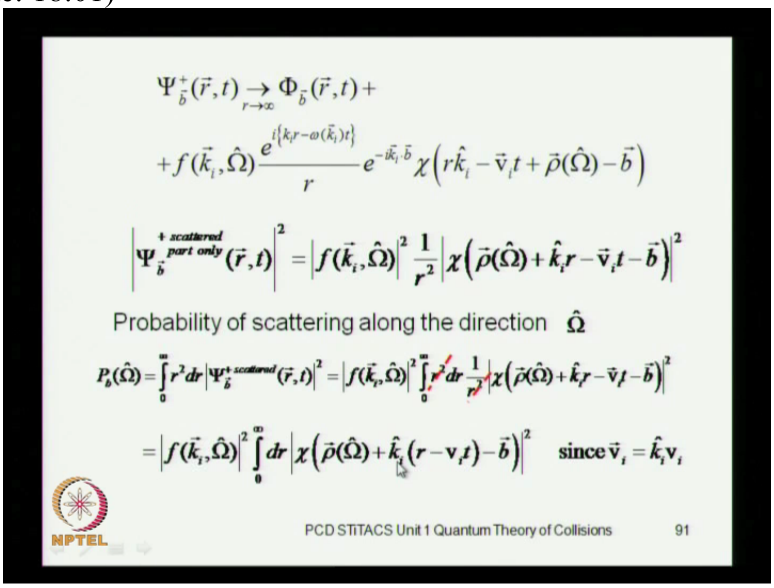

So that is what we have got. Now if you take the modulus square of a wave function what do you get you get the probability density right. You get, it is like Psi star Psi, so you take the probability density corresponding to the scattered wave function just the scattered path. So, this is the same wave function with a superscript plus corresponding to the outgoing wave boundary condition.

But only the scattered part this is written over here as a superscript scattered part only. So, this is the modulus square of this term then you have got 1 over r square modulus squared of this term which will give you unity, modulus squared of this term which will also give you unity and then you get the square of the modulus of the shape function right.

So, these terms e to the i theta and this is another e the i theta type of thing these simply drop out when you take the square of the modulus because you multiply it by the complex conjugate. So, this is the probability density and how will you get the probability from this you have to integrate this over the distance right.
It is the probability of scattering in a particular angle at a particular angle omega right. Omega is a unit vector which gives you the direction in which the wave packet scatter and this is the probability density corresponding to that, so to get the probability itself you integrate over r going from 0 to infinity because that is the only variable which is less left okay.

You have got three degrees of freedom in space, two degrees are contained in omega which is a unit vector right the in the spherical polar coordinate system you have got r theta Phi so theta and Phi already go into this, this definition of the unit vector and the integration in the third degree of freedom is over r going from 0 to infinity r square dr.

This is the element radial element integration element and then you have got the square of the modulus of this scattered part. Which we know is given by this square of the scattering amplitude. You have got this matrix element, this radial element here r square dr, you got this 1 over r square and the square of this, of which the r square will cancel easily okay.

And then you are left with modulus square of the scattering amplitude and integration from 0 to infinity dr of this shape function. Now I do not know if some of you already see the result emerging in advance but the only other thing that I have done over here is I have combined these two terms.

Because vi is the direction of the incident velocity which is the same as the incident momentum. So, I have combined these two terms, so that the unit vector ki is common to both and they multiply r - vi t, which are the corresponding magnitudes okay that is the only thing that we have done over here.
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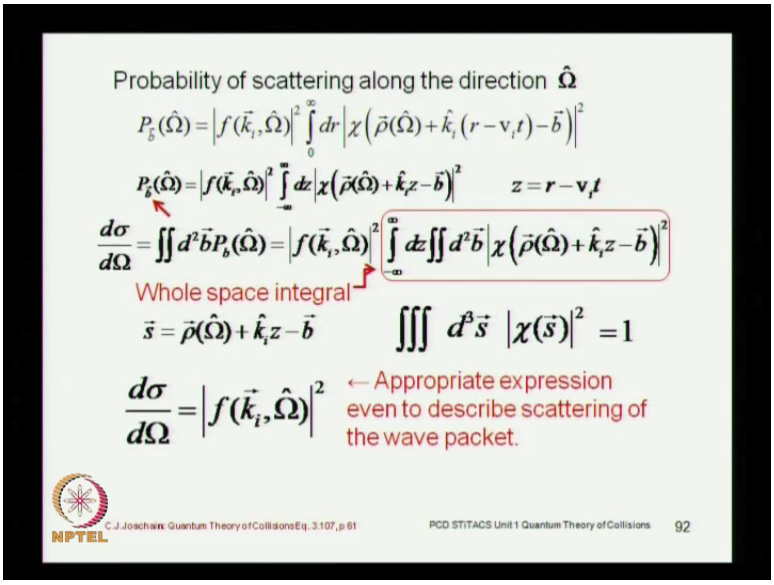

So, this is the probability of scattering along a particular direction in space which is given by the unit vector omega. And if you now change the integration variable from r to z okay, now what is the relation between z and r, z is r cosine theta but cos theta goes from -1 to +1. So, the range of integration for z will be minus infinity to plus infinity corresponding to the range 0 to infinity of the distance r.

So, you have got integration over z this is just a change in variable from r to z range of integration will be minus infinity to plus infinity and this is the probability of scattering along the direction omega but what is the original wave packet that you considered. You consider a wave packet at a particular impact parameter b right.

So, to get the complete probability of scattering in this direction you must integrate over all the impact parameters. And all the impact parameters the impact parameters are in a plane which is orthogonal to the propagation of the incident beam right. So, you have to carry out an integration over b to get the complete probability of scattering along the direction of omega having taken into account all the possible impact parameters.

So, you now integrate over the impact parameter b, so there are, the impact parameter in this plane, so it has got only two degrees of freedom, so there is a double integration you can write it in Cartesian coordinates or any coordinate system it does not matter. But basically it is a double integration corresponding to the two degrees of freedom in this plane right.

So, there is this double integration corresponding to integration over the impact parameter b. This is independent of b and then you have got integration over z going from minus infinity to plus infinity and the double integration over the impact parameter. Now what kind of integration do you have here? You have a triple integral.

Yes (Question time: 24:01) we are writing r - vi t = z, yeah so how is this limit changing from 0 to infinity to minus infinity to plus infinity. See essentially means, essentially what you are doing is integration over whole space, and essentially we are not taking the whole space, we taking only the odd integration, correct because it is probability of scattering in a particular direction right.

If you take the z axis along that direction whatever it is like omega, you can orient a new Cartesian coordinate system with a z axis along that direction. And what will be the range of z, z because r goes from 0 to infinity and the only way you can occupy the whole space by the z variable is to let it change from minus infinity to plus infinity because z going from 0 to infinity will be only half the region.

So, that is what you have got over here, so you got z going from minus infinity to plus infinity and this is integration over this plane. Now together with integration over z and b you essentially have integration over whole space because you have bought direction one direction and two directions in a plane orthogonal to that, it is essentially a whole space integral you can write it.

You can do some algebra if you like transform it from x, y, z to r theta Phi or r theta Phi to x, y, z, whatever it is no matter what variables, what coordinate system you use, your results are going to be independent of the coordinate system, your integration is going to be independent of the coordinate system. Essentially you have a whole space integral and you can express this integral as a triple integral.

So, that you occupy the whole space for a given argument s which is given by the complete argument of the shape function Chi. And this is the triple integral that you have which is the whole space integral. What did we, what do we know about it? We already know what this integral is; we have discussed this in an earlier class. That we have chosen the normalization in an earlier class such that the integration of this shape function = 1.
So, you do not even have to evaluate it, it just does not matter what the details are; what the detailed shape function? How it explicitly depends on z or r omega is not relevant at all it is a whole space integration of the modular square of the shape function and it must go to unity because that is how it has been chosen. So, now we have the result because on the left hand side you have got the differential cross section in a particular solid angle d omega right.

And this differential cross section is equal to the square of this modulus of the complex amplitude multiplied by this triple integral which is equal to unity. In other words d sigma by d omega is equal to the square of the complex matrix amplitude. Now this result which we have seen earlier for pure mono energetic waves, we now confirm, convince ourselves that this is a correct.

It provides a correct description of scattering even if you are dealing with wave packets in which they are not all the contributing waves are not strictly mono energetic even if there is a little bit of spread. This relation is quite appropriate and we can therefore continue to use it without worrying about the fact that we are using with a realistic wave packet. But then most of the analysis as we will carry out will be in fact in terms of pure waves okay.
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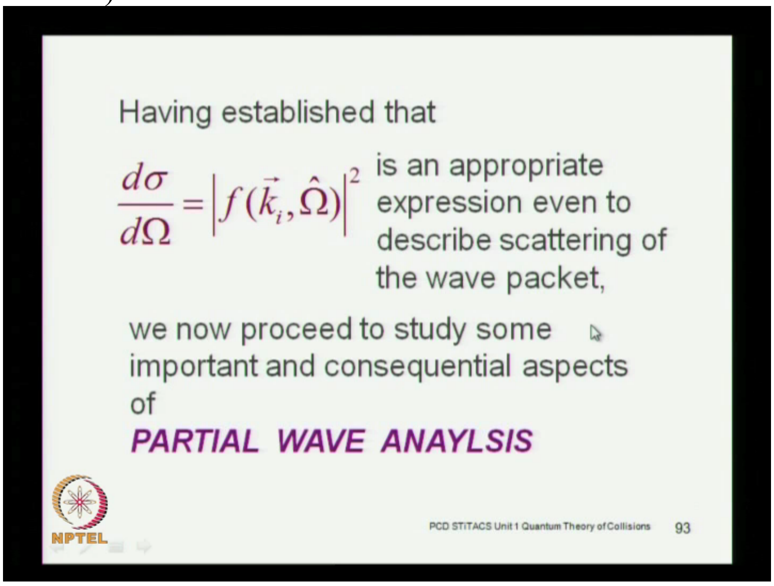

Because it provides a simple; you know analysis and for that we make use of techniques and partial wave analysis. So, this result we have seen this is appropriate for wave packet scattering as well and we will now focus on partial wave analysis method. There is a single mono energetic plane wave which is incident that we will now consider.
And then we can break this up into partial wave's error going from 0 to infinity. These are the partial waves and we have discussed this earlier, so I will quickly remind you of some of the fundamental relations in this expansion. So, this is the incident plane wave which is a strict mono energetic wave it is presented by e to the ik dot r.
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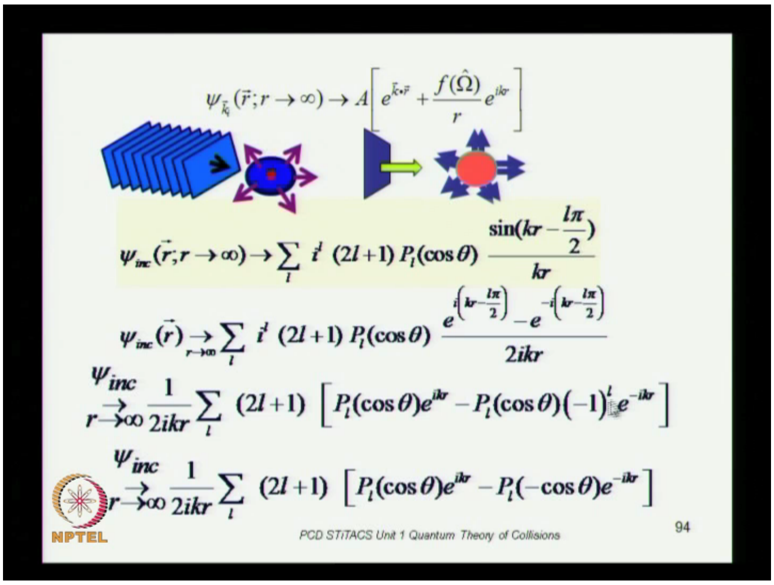

This is the scattering amplitude without going wave boundary conditions. So, the incident wave has this asymptotic form which we have seen and various books use different asymptotic forms. Also in the same book you will find alternative equivalent expressions. So, it is good idea to remind ourselves of what these alternate forms are and I will quickly remind you of those forms.

So, this is one of the forms that you have used earlier. You have also written this in terms of the spherical outgoing waves and the spherical in going wave's right. And you notice that there is, from where is this l pi by 2 coming; l pi by 2 is, pi by 2 is coming is because whenever you go from one partial wave to the next there is a further phase shift of pi by 2.

So, when you do it l times it becomes l pi by 2. So, this is another form in which you meet the incident plane wave you can take the Pl cos theta, the legendary polynomial as a common factor which multiplies the first term as well as the second term and write it in some other equivalent forms.

You play with these terms e to the -il pi by 2 and e to the -l il pi. And you can write this as -1 to the l, you can also combine this -1 to the power l together with this legendre polynomial. You get a legendary polynomial corresponding to minus cos theta over here. So, these are various equivalent forms that you have seen.
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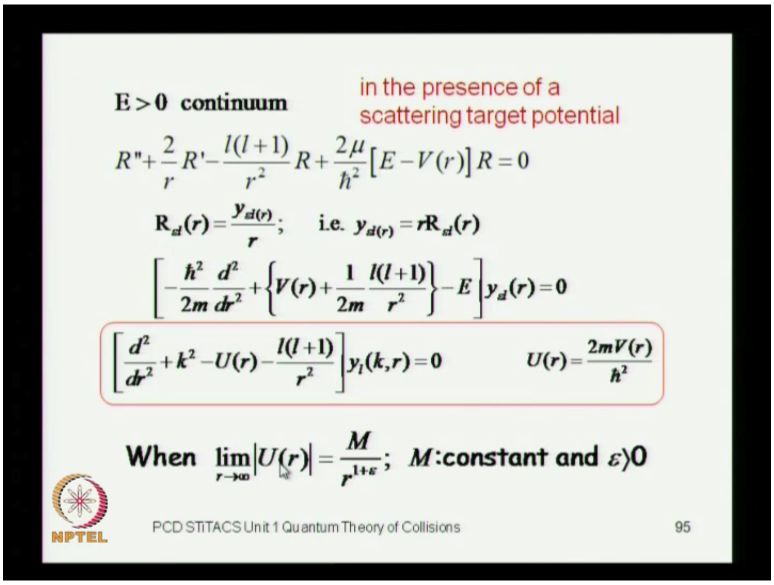

And then when you consider the total solution in the presence of a scattering target potential. You can write this radial part as y over r and then you deal with an effective potential and find the solution for this y of r. This is when this is divided by r you get the complete radial function. So, you have an effective potential which is made up of the physical potential Vr and the centrifugal term.

So, together you have these terms and this is reduced potential as is sometimes it is called all you have done is to multiply it by 2m over h cross square. So, that you can write this in a somewhat simpler form without writing carrying these h cross and m terms in all the terms. So, instead of that this is just a simple compact way of writing this by introducing this reduced potential.

We have also discussed that when this effective potential falls faster than the Coulomb potential and we have discussed why this condition has to be satisfied that under the conditions that this potential falls faster than the Coulomb potential.

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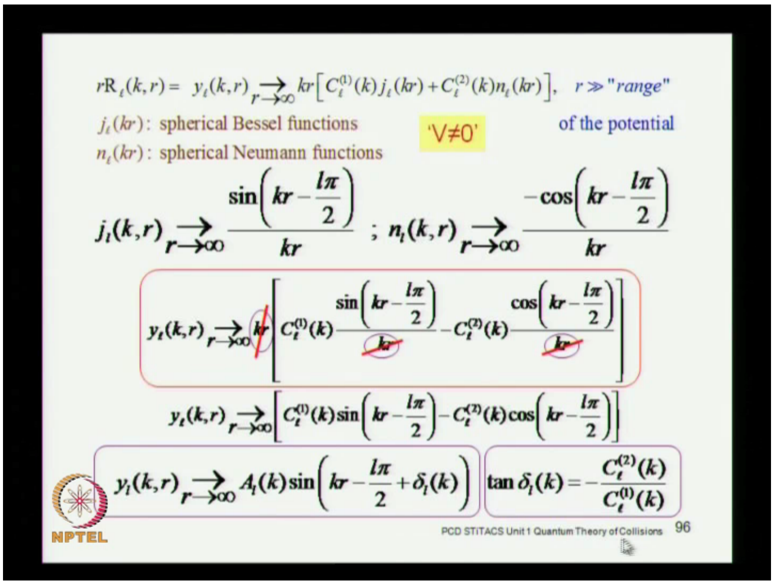

You can solve this rather easily and the solution is a linear combination of the spherical Bessel function and the spherical Neumann function. It can of course be written as a linear combination of any two linearly independent basis functions. But here we have chosen to do it in terms of the spherical Bessel and the Neumann functions.

And our interest is in the region where you are going to keep the detector so well outside the range of the scattering potential. And these are the asymptotic forms of the Bessel and Neumann functions, so the Bessel function goes as sine over kr and the Neumann function goes as -cosine over kr with these arguments okay.

The argument kr is shifted by l pi by 2 as we know and in terms of these Bessel functions, in terms of the asymptotic forms of these Bessel functions. This is the solution for y, the solution for r will be y divided by r. So, right here you find that the kr in the numerator here can cancel the kr in the denominator.

So, you write this in a somewhat simple form without the kr and this is your asymptotic form for the y function and now you can define the scattering phase shift from this ratio of these coefficients and that appears over here. So, we have seen these forms earlier also. (Question time: 33:59 not Audible) –cosine kr by l pi by 2;

These are very own properties of the Bessel and Neumann functions okay, you can set up the Bessel equation take its linearly independent solutions. There are two linearly independent solutions one is the Bessel the other is Neumann. If you look at the asymptotic forms these are the forms that you get.

You can also write it in terms of the Hankel functions, if you like, so you can make linear combinations of the Bessel and the Neumann okay. So, it does not matter what basis pair you are using as long as it is a linearly independent function because any general solution you can always write in terms of any pair of linearly independent based function.

So, you can write it in terms of the Bessel and the Neumann or the Hankel 1 and the Hankel 2 okay. So, this is the scattering phase shift and these expressions we have met earlier and this is just a quick recapitulation.

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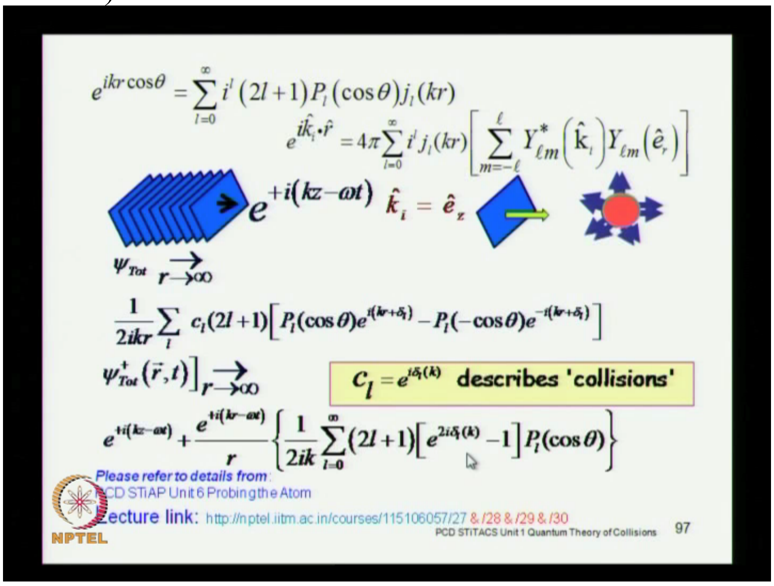

So, that we can continue with the partial wave analysis, we have done this in some details in the previous course and these are the four lectures lecture number 27, 28, 29 and 30 in unit 6 of our previous course and all the details are there. And in this we know, we have discussed that you choose the coefficient cl according to outgoing wave boundary conditions to describe collisions.

And I will not repeat that discussion over here but only refer you back to these lectures which we have already discussed this particular factor and with this you have the Faxen Holtzmark's resolution of the scattering amplitude in which the primary quantity of interest is the scattering phase shift okay. So, this is, these are some of the things that I wanted to quickly remind you, so that we can continue with the partial wave analysis in our subsequent classes.

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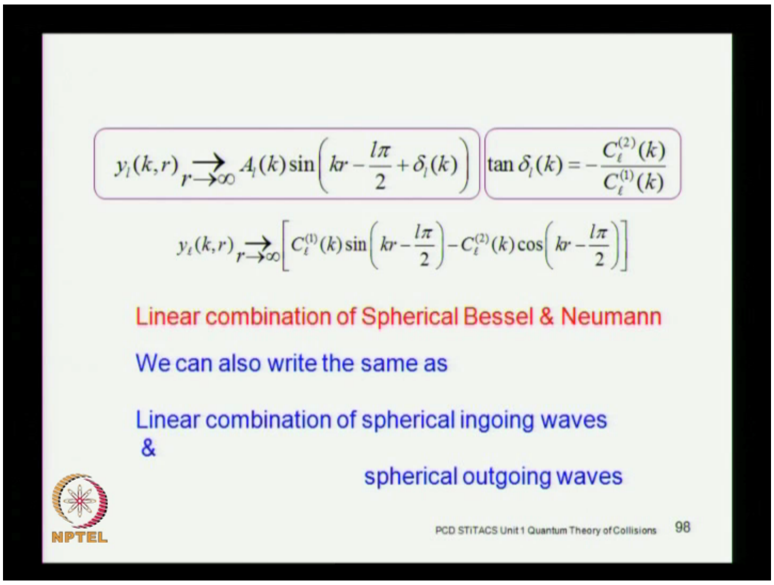

Essentially what we have done is to describe them in terms of the spherical Bessel and the Neumann functions. It is also a good idea to write them in terms of spherical in going waves and outgoing waves. And that is where we get some sort of insight when you write it in terms of the ingoing and outgoing waves.

Because those are very physical you know although mathematically any base pair is equivalent. But the spherical outgoing wave really corresponds to the scattered part. So, from the physical point of view it is more useful to write these solutions in terms of the spherical ingoing and outgoing waves.

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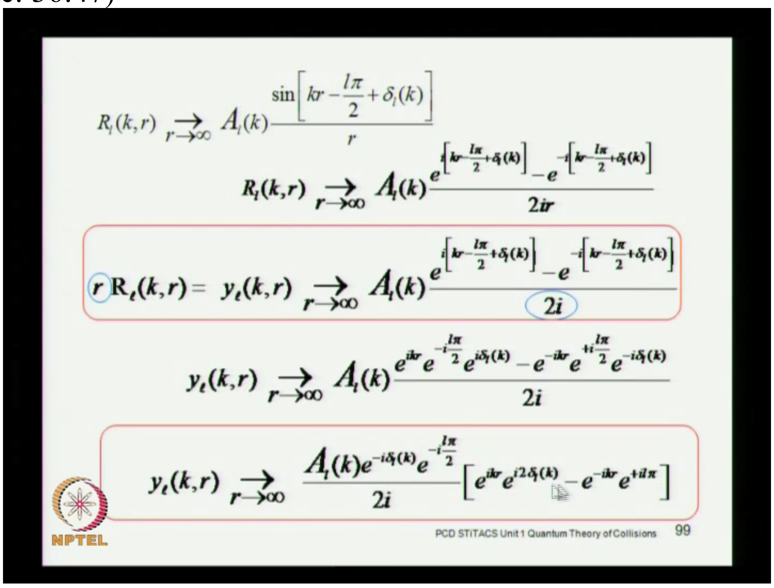

So, this is the description in terms of the spherical ingoing and outgoing waves of the radial function right. So, this is the complete radial function r, so little r times capital R is this function y which we have been working with and since you multiply this capital R with r your instead of this 2ir in the denominator, you have only 2i. So, the r is over here, so this is the function y.

And you can look at these phases keep track of each term and essentially you can factor out some of the terms. Inside you have got a linear superposition of a spherical outgoing wave which is e to the ikr scaled by this scattering phase shift. And this is the spherical in going wave multiplied by e to the il pi, which is a constant right. Its value depends on the value of l for each partial wave it will be different.

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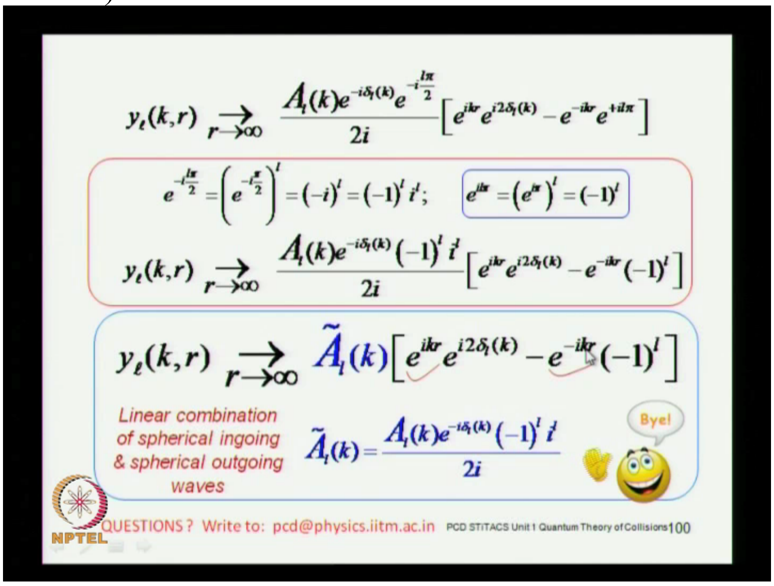

So, e to the il pi is -1 to the power l and it will be either odd or even depending on the value of l right, because l is an integer goes as 0, 1, 2, 3, etcetera. So, this is e to the il pi over here and this solution y is now given by this whole amplitude together with this 1 over 2i is what gives you the amplitude.

Then you have e to the ik r multiplied by this phase factor with the scattering phase shift and the spherical in going wave multiplying -1 to the l which determines the phase of the ingoing wave. So, this whole factor is now what is written as again an energy dependent normalization together with these additional phase factors okay.

So, all of these are additional terms, so you define a new normalization which is A tilde basically there is nothing new in it, it is just a short description of writing all of these terms. So, this is your A tilde and this is the way you write the solution y in terms of spherical outgoing wave and the spherical in going wave and that gives us a common expression of the solution to the scattering problem.

And we will take it from here in the next class essentially we have written the solution as a linear combination of spherical ingoing and outgoing wave. And like I mentioned mathematically it is completely equivalent to writing in terms of the Bessel function and the Neumann function or the Hankel functions.

But this is the form which will reveal some of the physical properties rather nicely. So, we will take it from here in the next class. Any question if not goodbye for now.