Select/Special Topics in 'Theory of Atomic Collisions and Spectroscopy'
Prof. P.C. Deshmukh
Department of Physics
Indian Institute of Technology-Madras

Lecture 05
Quantum Theory of collisions- Differential Scattering Cross Section

Greetings, we are, we will resume our discussion on the differential scattering cross section and we had considered a plane incident wave, mono energetic pure plane incident wave. For which we know that the differential cross section goes as the square modulus square of the scattering amplitude.

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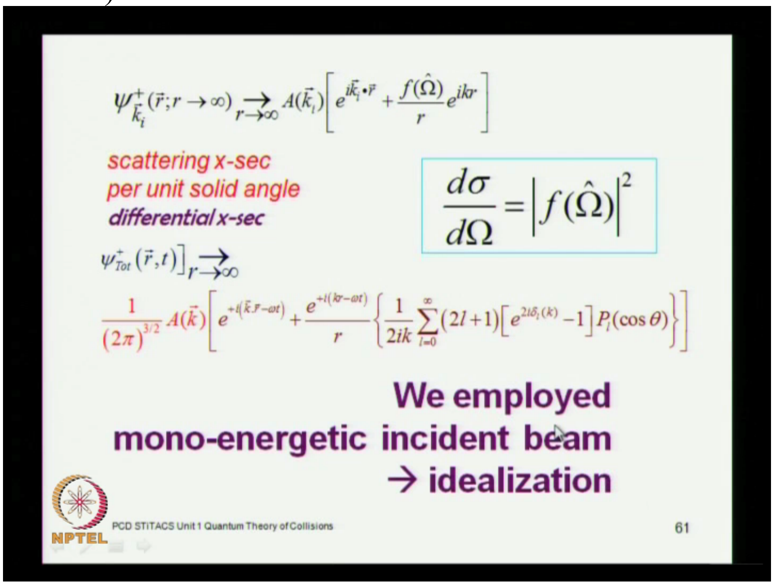

And what we had employed to arrive at this expression was a strictly mono energetic wave which we resolved into partial waves right. So, this was the resolution which we employed and then we got the scattering phase shifts and so on. And then we got the expression that the differential scattering cross section per unit solid angle d sigma by d omega is given by the modular square of the scattering amplitude.

Now this is clearly an idealization okay, in a real situation you will have not just a pure single momentum vector. But you will have a collection of momentum vectors and they will all be in the neighbourhood of a given energy but not exactly at that energy. And they will not be exactly at the same momentum vector because momentum is h cross k. So, there will be a little bit of spread.

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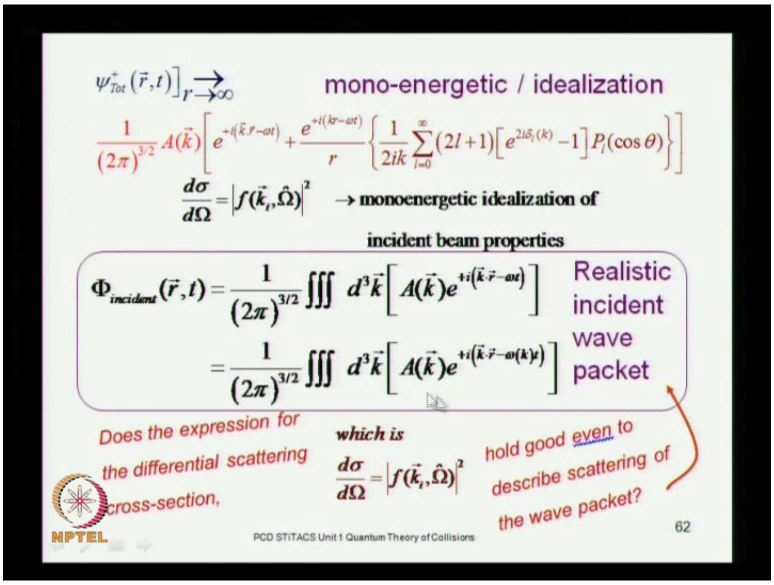

So, this idealization is not the real situation that you expect to meet in a scattering experiment. A real incident wave will then be a superposition of plane waves of this kind okay. Because there will be several of them and this omega which is frequency will in fact depend on k according to whatever is that dispersion relation. So, there will be a little bit of k dependence of omega.

So, you will have to take that into account and ask the question if this expression d sigma by d omega equal to squared of modulus of the scattering amplitude. Is this expression valid also for a realistic incident wave packet as it is for a strict ideal mono energetic wave? So, that is the question that we began to discuss in our previous class. And we will continue our discussion of this particular point.

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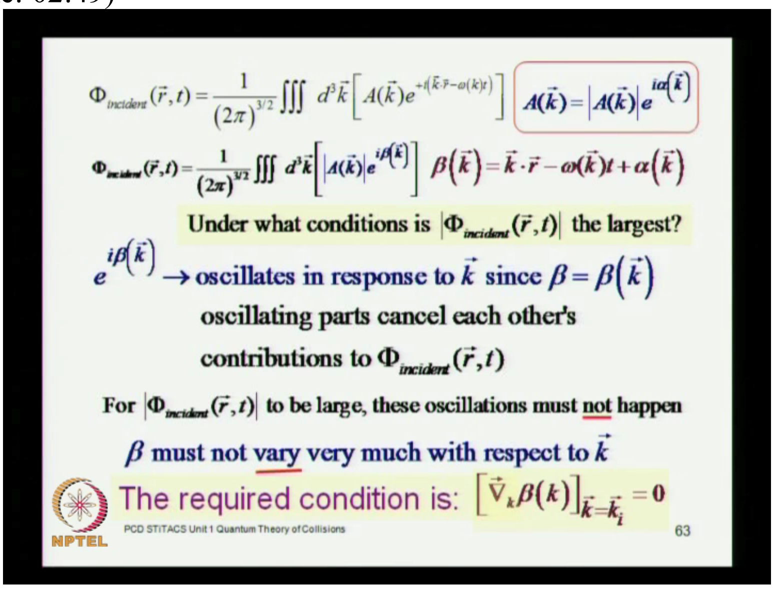

So, this is the incident wave which is a superposition of waves of the previous kind. This amplitude in general is complex so it will have a real part and a phase part okay. So, complex number you can always write as Rho e to the i theta, where Rho is the size of that particular complex number right and alpha will be the phase. So, you can write this in terms of this Rho e to the i theta kind of structure.

And with this structure you have the phase which consists of this k dot r -omega t, this phase must be expanded to include this k dependence of alpha which is coming from the phase of this complex amplitude A. And you have a net phase which is k dot r -omega + alpha okay, so this is the total phase of this particular term.

Now the question is if you have the incident wave packet which is reaching the target and so that you know there is an encounter and scattering takes place. Now you do know that when you have a number of waves when they reach a certain destination like if you have waves coming in from a source, there is a screen it may have some holes even if it is an incident optical wave, if you like right.

There is this incident you know if there are holes in the screen and then you have got a detector screen then the intensity that you find on any point on the detector screen is just a superposition of what you get from all of these holes right. So essentially all of these waves have to have a superposition principle which they must observe, waves do observe.

Now this is the fundamental principle of linear superposition which is applicable to all wave phenomena. And we also know from the superposition formalism that if waves with equal amplitudes reach a particular point of the detector in opposite phases they can kill each other or else they can augment each other right.

So, there will be some sort of interference and they could actually in principle kill each other and since you are performing a scattering experiment in which the incident wave packet reaches the target. You ask the question what is the condition under which, this incident wave will be the largest. So that these phase factors because this is oscillatory beta k and depending on k beta will change.

So, for different values of k it is possible that these oscillations cancel each other and you will not have a net resulting, resultant intensity. So, the condition that this Phi is the largest is that these oscillations should not kill each other. In other words this particular condition which is leading to the cancellation, cancellation is taking place because beta is a function of k.

And this condition should not be satisfied in other words because the cancellation coming is coming because the different components in the superposition have got a net phase which depends on k. The condition for non cancellation is that these oscillations should not happen and therefore beta should not change very much with k.

And if beta is not to change very much with k what it means is that the gradient of beta with respect to k must vanish. So, that is the mathematical condition that must be satisfied so that you have a net wave packet right. So, this is the condition that you are looking for and let us ask if this condition is satisfied.

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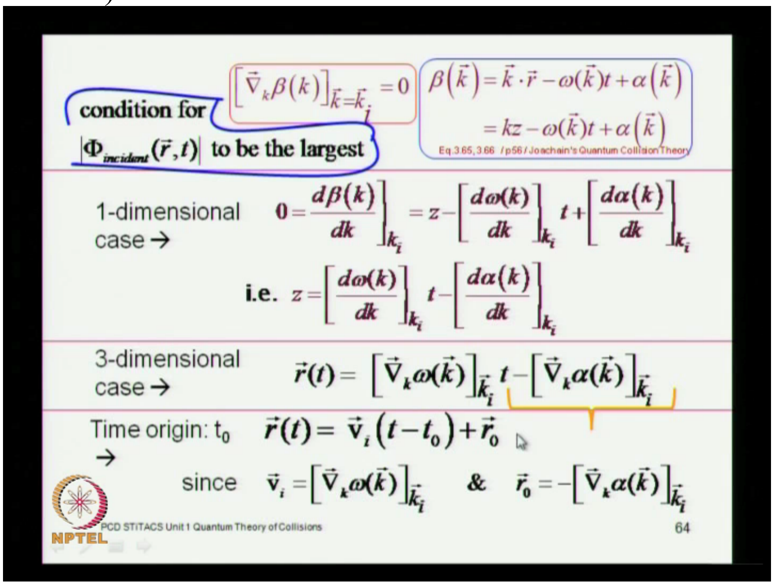

So, this is the condition for the incident wave packet to be the largest. This condition is that the beta gradient must vanish gradient with respect to k must vanish. Beta is given by this k dot r -omega t +alpha, as we have seen k dot r is let us say kz that is by the choice of the z axis of the Cartesian coordinate system or cosine theta is what we call as z okay.

So, that is the orientation of the polar axis. And if this were just a one dimensional problem our condition for Phi incident to be the largest would be that the derivative of beta with k vanishes in one dimension right. So, what is the derivative of beta with k, you get a term from here then you get -d omega by dk and then you get d alpha by dk.

And these derivatives you evaluate as at a certain incident momentum okay. So, this is the condition that you would get in one dimension and you can rewrite this as z = d omega by dk times t minus the derivative of alpha with respect to k. So, that is your condition which must be satisfied.

And you can easily generalize it to three dimensions by writing instead of this Cartesian components z, you write the full position vector instead of this derivative, this derivative and the second derivative, the derivative of alpha you use the corresponding gradients with respect to k. So, that is the automatic you know mathematical generalization from one dimension to three dimensions.

So, this is your condition that the position vector is given by the, this term which you will recognize. This is the gradient of the circular frequency omega and you know that this is the velocity of the packet right. So, you have the velocity of the packet which is appearing here is the gradient of omega with respect to k. And this is vi you can shift the time origin to t0, whatever it is. So, instead of t you have got t - t0.

So, you have the position vector equal to velocity times instead of just time t, you have t - t0. And this minus gradient of alpha is what you call as r0 that is obviously a position vector it has got the dimensions of length. And this is how you define a certain r0, this r0 is related to the gradient of this phase alpha. So, this is defined along with a minus sign which is why you get a plus sign here. So, let us use this result in our expression.

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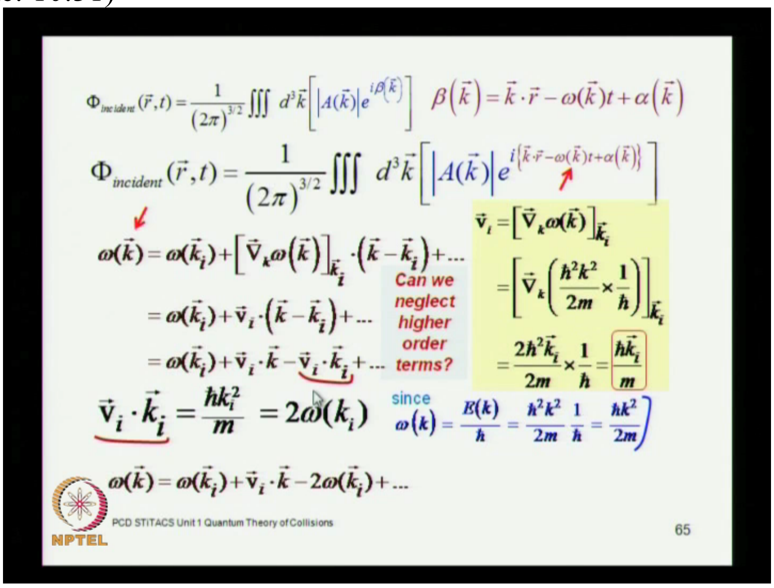

And these are our, this is the complete phase and we now look at how omega appends on k because the gradient of omega has already appeared in our expression right. So, the gradient of omega the group velocity will depend on what kind of k dependence the circle of frequency omega has okay. So let us write this expression, so let us expand omega k about a certain incident direction ki momentum vector.

And this is the first term, leading term plus the gradient of omega with respect to k at that particular value of the momentum which is ki times the difference from that momentum vector that is the first term. And then you will get higher order terms coming from second derivative, third derivative and so on right. So for the time being let us ignore those higher order terms.

And we are going to of course ask the question, if we can neglect the higher order terms. So, we will discuss that question in a little while. In the meantime let us see what form this takes. So, the gradient of omega is the velocity so you have got the dot product of this velocity with this difference in momentum vector in units of h cross. And you get two terms one is vi dot k, the other is - of vi dot ki, which is here.

So, you have three terms over here for omega and we do know in fact that omega, what depends, how it depends on k omega is e over h cross. So, it is h cross square k square over 2m, so if you take the gradient of this quantity okay h cross square k square over 2m into 1 over h cross which is 1 omega is. So, what do you get, you get the product of h cross over m and the k vector right. This is just the particle velocity.

So, that is the group velocity and the particle velocity they are the same. So, we know what omega is in terms of k. So, we get this group velocity which is equal to the particle velocity and you can use this form h cross ki by m to get this term, what is this vi dot ki, but vi is a along ki. So, you get a ki square multiplied by h cross over m. So, you have this term h cross ki square over em and what is h cross k square by m.

It is twice this value this is h cross k squared over 2m, this is h cross k square over m. So, this is twice omega so that is what you get right. So, you can put twice omega instead of vi dot ki and that gives you an expression for omega in terms of the momentum vector k which is omega as a function of k is given by this first term omega ki. Then you have got the second term which is vi dot k.

You got the third term which we know is with this minus sign, it because minus twice omega ki and there is a minus twice omega here, there is a plus omega ki over here. So, these two will give you a minus omega and that is the net result that we get of course assuming that higher order terms are neglected and we will come back to this question okay.
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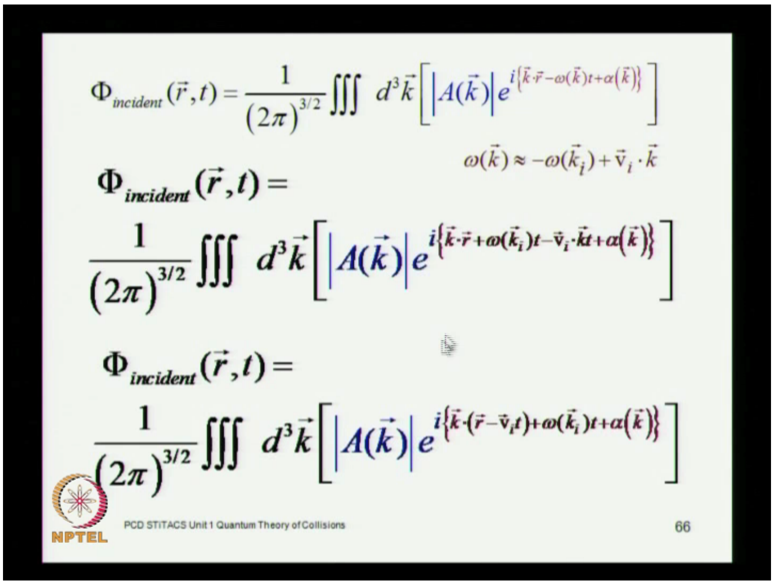

So, this is your expression for the k dependence of the circular frequency. And now you put this omega into t in terms of these two terms - omega into t + vi dot k into t. So, vi dot k into t, but there is a minus sign here, so you get + omega into t - vi dot k into t right. So, that is a mere substitution of these two terms over here.

And then you can combine the terms r - vi dot k, so you have got the vi dot k is coming in the second term and this is multiplied by t. So, you have got a k dot r - vi t, you have got omega ki t coming from here and the alpha k coming from here right.

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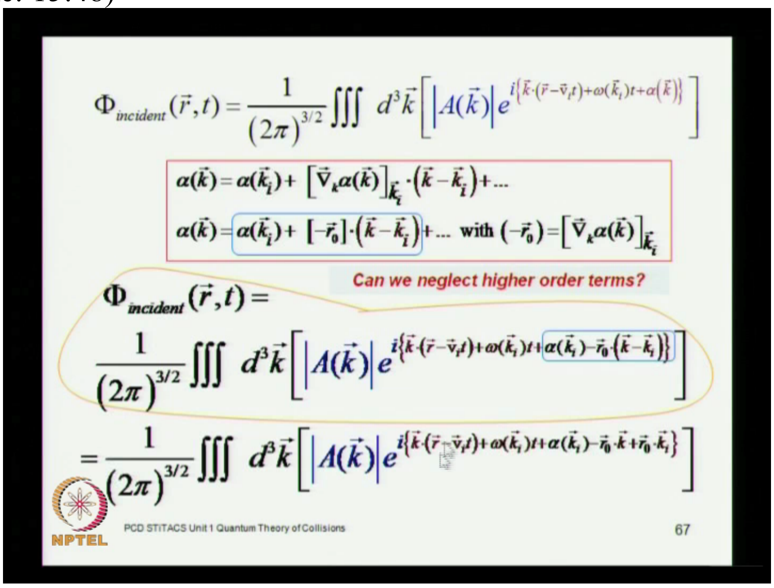

So, we bring it up to the top of the next slide and you also now have to consider in as much as you considered the momentum dependence of the circle of frequency, you also had the gradient of alpha okay. Now what is the gradient of alpha, so this alpha also depends on k. So, you can expand it about the initial a particular momentum vector ki which is the incident momentum vector, i is the subscript corresponding to the incident momentum vector.

And if you expand it about this you get a leading term plus the gradient with its scalar product with the difference in the two momentum vectors in units of h cross plus higher order terms and again you will ask if the higher order terms can be neglected. So, it is the same question but we will answer the two questions together.

So, we already have identified this as our -r0, the gradient of alpha we introduce r0, it has got the dimensions of length and we have defined our r0 with a negative sign here. So, we will write this as negative ro. And along with this you have these two terms over here; this alpha k is replaced by these two terms first term and this r0 dot k – ki, with a negative sign.So, these are the two terms that you should put in, in your complete wave packet for the incident beam of particles.

So, there are a number of terms which go into the phase all of these together constitute the phase and they have only been separated over here. So, these two terms r0 dot k is here and then r0 dot ki is here, with a plus sign okay. Because there is a minus sign here is also a minus sign here so it comes with a plus sign here. So, this is your complete expression for the incident wave packet.

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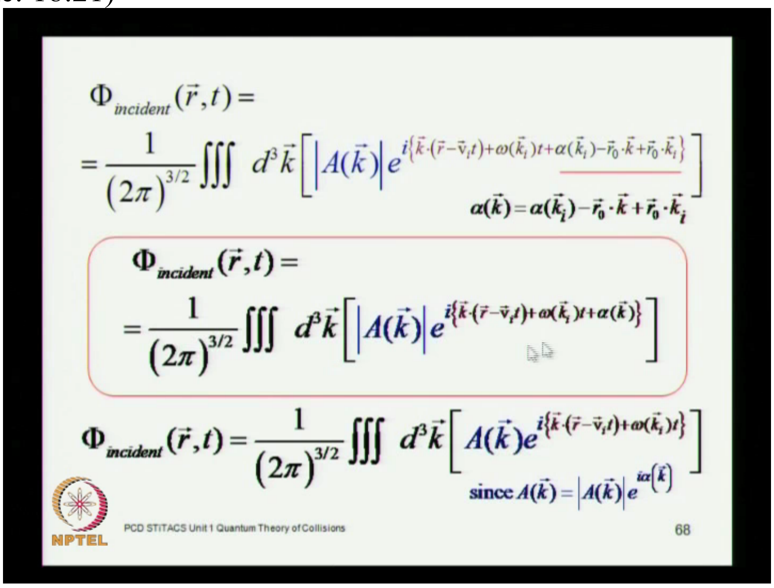

We bring it to the top of this right now and what do we, have we have the sum of these terms which is nothing but alpha k and we can rewrite in an equivalent form in a slightly compact notation. We first separated it, now we recombine it just to write it in a more compact form. But we separate it to recognize how the gradient of alpha is coming into the picture okay.

So this is an equivalent form of the incident wave packet and we recombine this in the original term because this modulus of A into e to the i alpha is what you had for the complex amplitude which scaled the different momentum dependent plane waves. So, it is just a recombination of these terms to see keep track of what the phases are.

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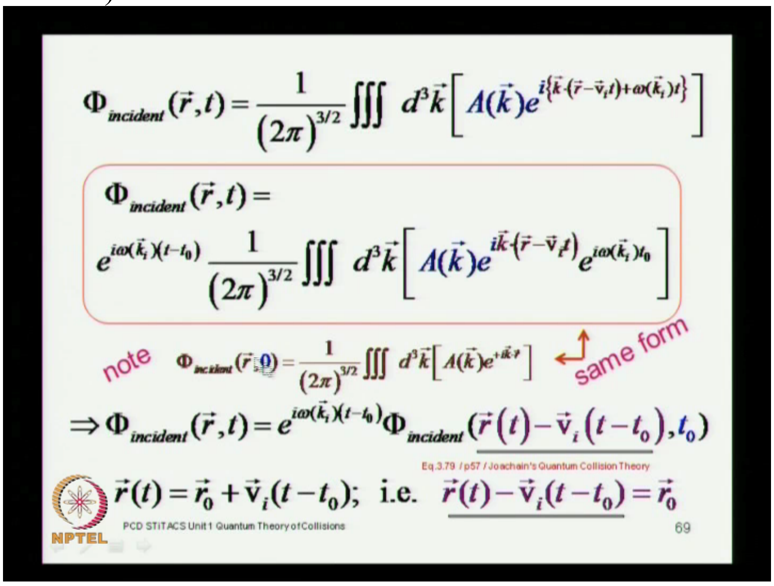

Having done this you factor out e to the i omega t - t0 from the integrand because ki is a particular unique incident vector it is not changing so it is not a variable in the integrand, it is a constant under the integrand. So, you can take it out of the integration okay. So, this phase corresponding to the incident momentum vector is pulled out and this is t - t0.

There is already an omega t here and because there is a -t0 which is pulled out you must compensate for it by inserting it in the integral okay. Now if you put t = 0, in this you get the incident wave corresponding to t =0 okay and notice that these two are of the same form, they are exactly the same form. So, what you have in this red loop is something very similar to this with the difference that the time is shifted to t0.

And the position vector is also shifted because instead of e to the ik dot r you have got to the ik dot r - vi times t. So, depending on how much time has elapsed, the position has elapsed and except for that it is exactly the same way packet. There is no difference except for a shift in the time and a corresponding shift related to the position of the wave packet.

So, it is exactly the same form which means that you can write this incident wave packet at an arbitrary time in terms of an incident wave packet at time t0 by recognizing this r0 + vi t - t0 to be equal to r of t, because you have got r - vi t here, so this r – vi t is what you call as r0. And with this r0 you have got exactly the same wave packet it is only shifted.

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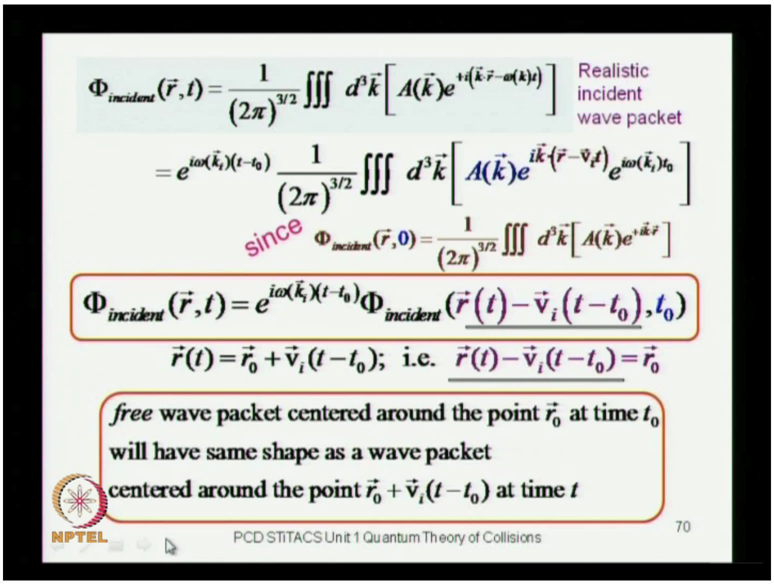

So, this is the realistic incident wave packet that we are working with that is the one that we started our discussion with. We factored out this term and we look at the value at t=0, recognize the identity in the two forms. And our essential conclusion from this is that you have got a freeway packet which is centered around r0 at time t0. It will have this exactly the same shape as a wave packet which was centered around a different point in space.

And where it is located depends on how much time has elapsed from the reference time t0. So, it will be the group velocity times t - t0, so it will be displaced by that and at a later time t. So, it will be exactly an identical so there is a shape function that you can expect to factor out from this analysis.

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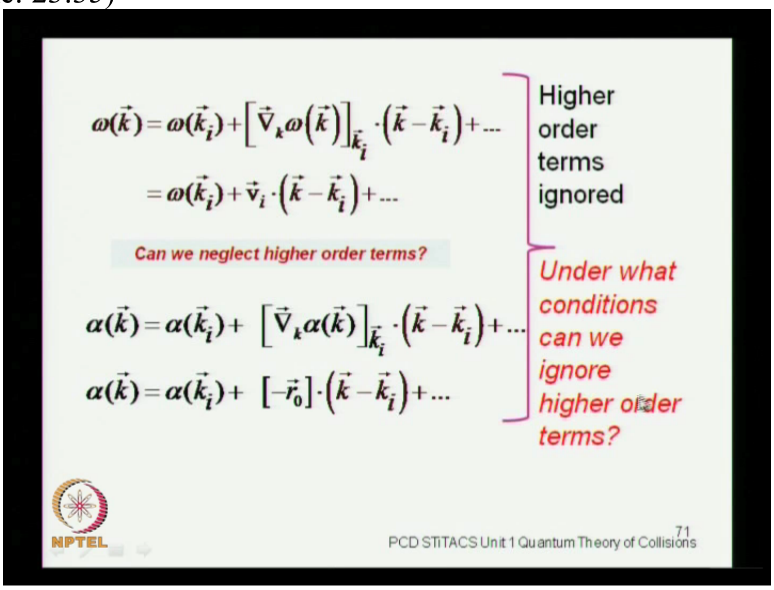

So, let us go back to the question that we had raised that we considered the momentum dependence of omega and there were additional terms that we could have considered coming from the second, third derivative etcetera which we neglected. We did the same with reference to the phase alpha which also had a momentum dependence.

And in both cases we have thrown out the higher order terms. We have ignored the higher order terms and we asked under what conditions can we ignore the higher order terms okay. This question we had raised and we need to answer this. So, let us take up this question and ask under what conditions can we ignore the higher order terms.

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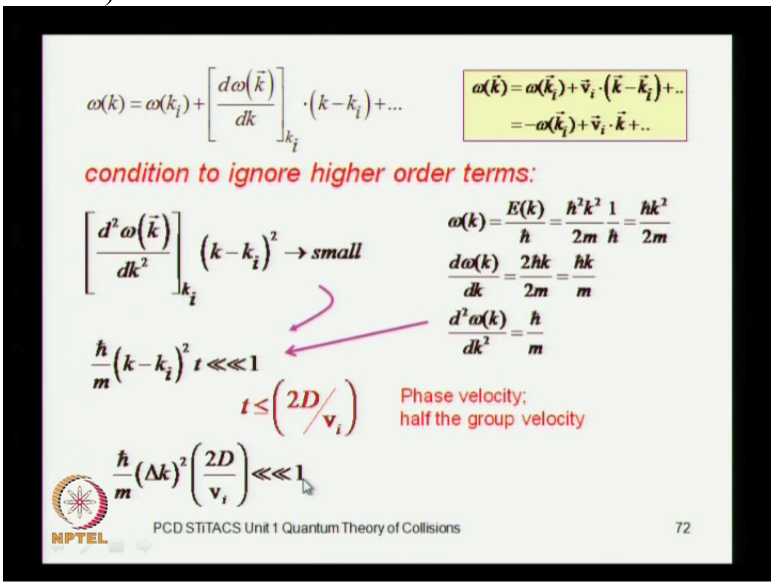

So, let us look at this expansion the condition to ignore the higher order term is that this, the first of the remaining terms which is ignored is the second order term. And if the second order term itself is small then by induction you can argue that the remaining terms can also be ignored. So let us be satisfied at just asking this question that under what condition can you ignore this second order term.

So let us look at the second order term the second order term which is the second derivative of omega with respect to k multiplied by the square of the difference k – ki, this is the second order term this must be small right. This is our condition, is this condition satisfied, that is whatever question amounts to. So, let us look at how omega depends on k, we know that it depends quadratically on k h cross k squared over 2m.

So, the first derivative goes with k and the second derivative is a constant which is h cross over m. So, instead of this second order term you can replace the second order term by h cross over m and you get h cross over m multiplied by this, this must be small and this multiplied by the time will give you a dimensionless number. That number must be equal to or it must be much smaller than unity.

So, that you can ignore its powers okay. Now what is the time scale we have in mind because this term obviously becomes large as t increases? And if t increases to 10 hours, 20 hours, 20 days, 20 months and 20 years, 20 million years and so on, it is going to grow right. And you cannot expect this to be less than 1. But what kinds of time scales are involved.

The kind of time scales that are involved depend on the velocities of these packets because the only time which is of interest to us is the time it would take for this packet to reach the detector okay. Once it reaches the detector you are done with the experiment okay and any further time is of no interest to you okay.

So, the time that you are really dealing with is how much time it will take to reach the detector. So, that depends on the kind of geometry you have set up for your apparatus in your laboratory and those are the physical time scales which are of importance in this mathematical relationship.

So, the mathematical relationship is that this product of h cross over m multiplied by the square of the difference in momentum in units of h cross times time must be less than 1. And this time will depend on how much time it takes to reach the detector and that distance in our geometry is capital D okay. But since the phase velocity is half the group velocity all you have to consider twice that distance right.

And if this t is less than or equal to twice distance by velocity then you are okay and this is what it amounts to. So, if this condition is satisfied that h cross over k this is delta as k squared and instead of this time we have this 2D over vi if this product is less than 1 then we are okay.

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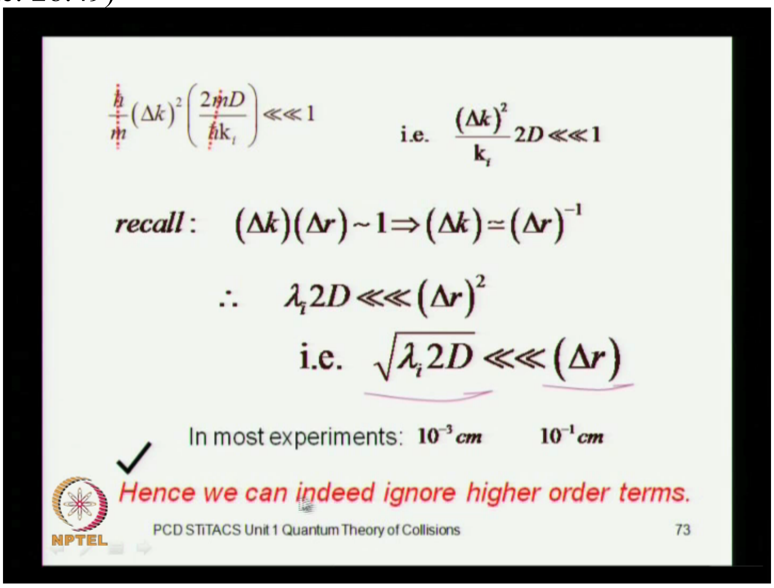

So, this is the condition depending on the distance okay, now this distance d is a laboratory parameter this is the distance from the target to the detector. So, now you notice that you have got an h cross square over m and an m over h cross here. So, these two terms cancel it cross over m into m over h cross or these two terms cancel.

And your condition now is delta k square over k into twice the distance should be much less than 1 that is what your condition boils down to. And this is the basic uncertainty that you are aware of the delta k times the uncertainty in the position that depends on how much the wave packet is delocalized. So this is of the order of 1, this product is of the order of 1.

So, we will just do an order of magnitude analysis. So, delta k is of the order of 1 over delta r, so this is delta k square, so this is 1 over delta r square right. It is 1 over delta r square. So, 1 over delta r square, I take to the right, so it becomes the square of delta r and here I have got one over k which is of the order of the wavelength okay, k is whole k is essentially 1 over lambda. So, you get from this delta k square on the left you get delta r square on the right.

And from this one over k you get a lambda. So, this condition is that lambda into twice D should be less than the square of delta r or the corresponding square roots should have the same inequality okay. And this is what sets the time scale because in a laboratory you have typically delta r which is of the order of one tenth of a centimetre. And this is of the order of one thousandth of a centimetre okay. Both are length scales.

These are the numbers that you deal with in most experiments or in some other experiments this may change but notice that 10 to the -3 is much smaller than 10 to the -1, it is a hundred times smaller. And this condition is therefore satisfied in an experimental scenario and therefore the condition that we needed to be satisfied. So, that we can grow the higher order terms is in fact satisfied in under laboratory conditions.

And we can ignore those terms, we can ignore the higher order terms happily this is satisfied and whatever expressions we had we can continue to employ them in our subsequent analysis okay.
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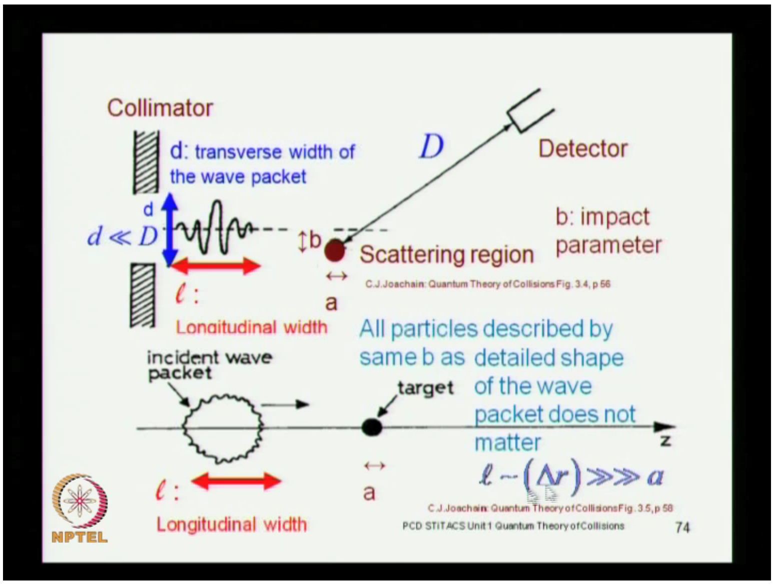

What have we got so this is the capital D that I was referring to, this is the length scale. Now this is the transfer's width of the wave packet, this is the longitudinal bit okay, that is the kind of scales which are involved. And it is this distance, if this distance is farther that is when the t will keep increasing. But how much D does it have to cover anyway okay.

So, it has to get to the detector and if it did that that depends on what is the longitudinal width. And these are the; this is the kind of geometry we have in picture you have got an incident wave which has got a certain spread which is the longitudinal width which is of the size of l. And then you have got a target which has got a certain tiny dimension of a.

And this length is of the; this is about the size of the uncertainty spread for our order of magnitude analysis. On the length scale which gives you the corresponding spread in the momentum which is inverse of this right. So, this is the picture that we have under consideration. The other thing you have to recognize is that depending on how it is set up you may not have the incident beam meet this target head on.

But there may be a little bit of you know distance because where it impacts the scattering region may not be exactly head on. There may be a little bit of displacement over there. So, there is a certain impact parameter that you may have to consider. And all particles described by the same b will have a similar shape.

So, the wave packet you know the exact detailed wave packet shape will really not matter. Because these distance is quite larger than the target okay. So, our analysis is quite on comfortable ground

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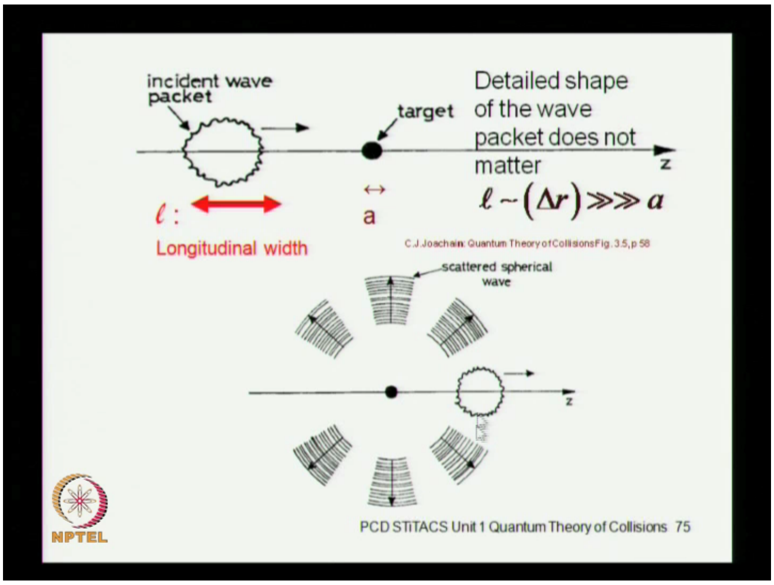

And detailed shape of the wave packet does not matter. So, you will have a scattered spherical outgoing wave and the incident wave. This net scattering solution as we know is a sum of the incident plane wave and a scattered outgoing wave. This diagram is from Joachain's book.

And you have got the net scattering solution which is a superposition of the incident wave plus the scattered waves okay as we had even for a mono energetic beam. So, that is what we considered already in details in some of our earlier discussions. But now we are trying to see how it gets modified, if it all is it gets modified.

Does it change your primary results when you are dealing with a realistic incident wave packet which is a superposition of plane waves around different momentum vectors? All momentum vectors which are very nearly the same but slightly different from a pure value of the incident momentum vector. So, there is a little bit of spread which is what generates this wave packet.

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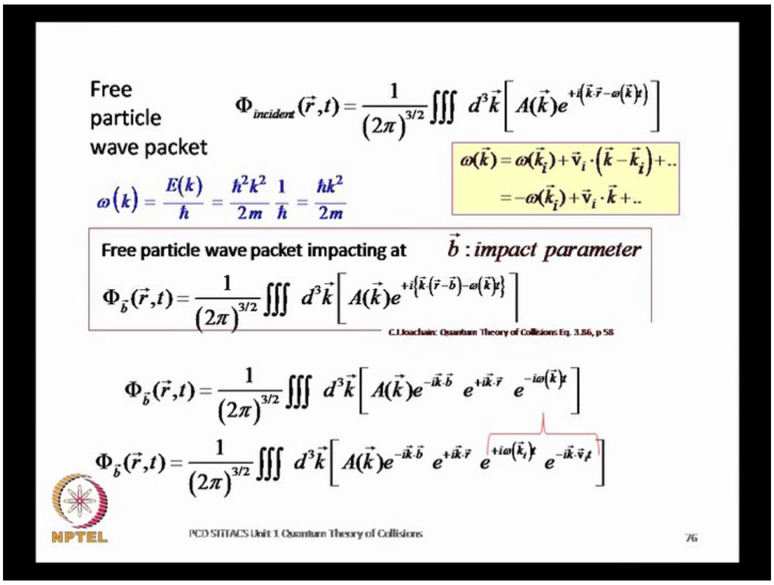

So, this is the free particle wave packet it is a superposition of free particles okay e to the ik dot r - omega t, is a plane wave, it is a free particle, if it is not to meet head on. But there is a displacement because of an impact parameter b, this r must be displaced by r - b okay. So, this is the same expression for a free particle wave packet. But it respects the impact parameter be right.

So, I have written this Phi with a subscript b and change this r to r - b other than that is the same thing. So, it is the incident free particle wave packet taking into account the impact parameter b. The phases then consist of e to the - ik dot b, e to the ik dot r and e to the - omega t. So, these are the three contributors to the phase okay.

This omega is depends on k so if you consider this dispersion because it is k-dependent you can write this omega in terms of these two terms which we have already found. So, this is the free particle incident wave packet.

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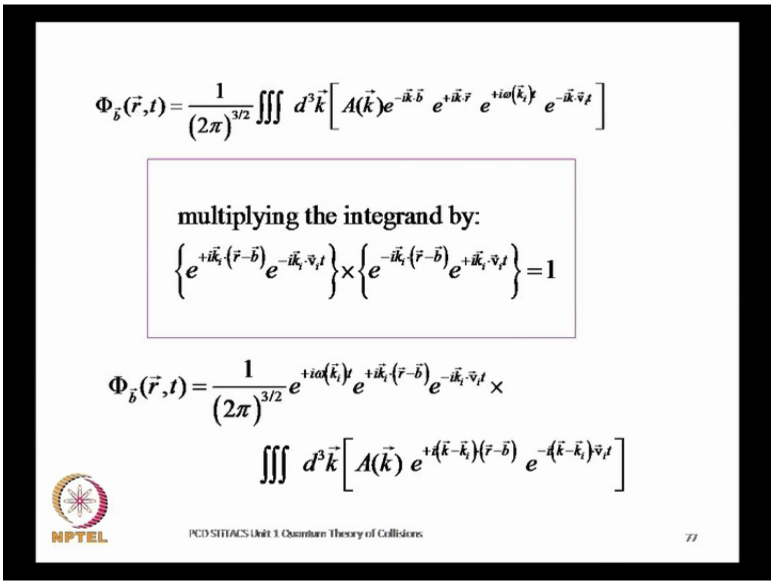

Now let us multiply the integrands by unity it never hurts right. And you can resolve this unity into these two factors okay. They are phase factors they are the same factors phase factors with a plus sign here and a minus sign here, is a minus sign here and a plus sign here, the same terms okay.

So, you multiply the integrand by 1 and then you factor out these three terms e to the i omega ki everything which does not depend on ki can be tabled out of the integration. Because the integration is over the variable k, so ki under that integration is a constant. And anything and everything that has got ki alone can be factored out the remaining term stay inside the integral.

And the net value of the integrand must be preserved which is guaranteed by factoring unity into these two factors. So, you factor out these three terms e to the i omega ki, e to the i ki dot r - b and e to the - i ki dot vi t. So, notice that what is pulled out of the integration has only ki and nothing else.

And having pull this out whatever remains inside is what will compensate for these factors so that you regenerate the original phase. So, it is just a little bit of very straightforward manipulation of the phase okay. Just r writing the phase in this particular fashion which is what will give us a very useful result.

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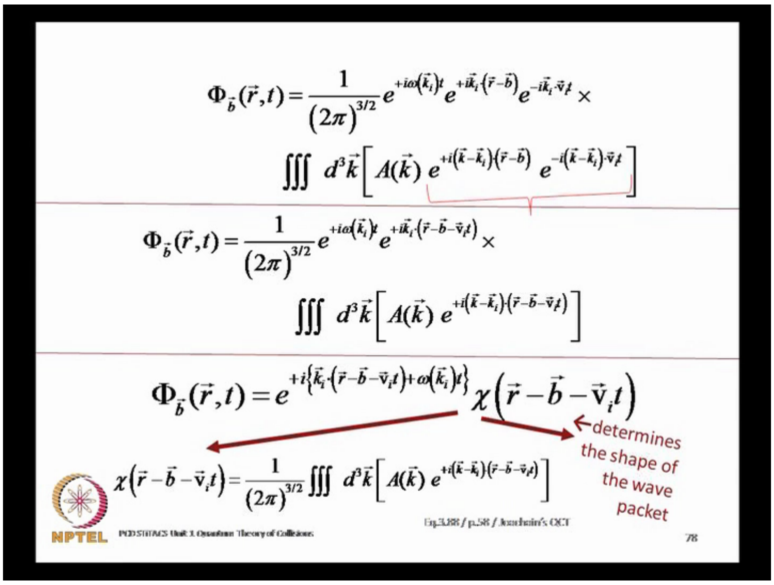

So, this is the same expression you have pulled out these ki dependent terms which are constants in k outside the integration the rest of the integral is here. And there is a k - ki in both of these terms so you combine them. So you k, have k - ki times r - b from this and vi t from this. So, you combine these two terms okay that makes it a little easy. So it is just a rearrangement of terms that we are doing here nothing very fancy.

And essentially what you find is that this is the factor this integration is what will have complete information about the shape of the wave packet. The remaining term is just a phase factor so this is the shape function okay. The entire shape is determined by this integral which is defined as 1 over 2pi to the power 3 by 2; this factor is absorbed in the definition of Chi.

And then you have got this triple integral in the momentum space of modulus of Ak and this phase factor which is a reconstruct of the original phase by factoring out appropriate pieces okay. So, what this rearrangement of the terms has allowed us to do is to introduce a shape function which is given by this Chi.

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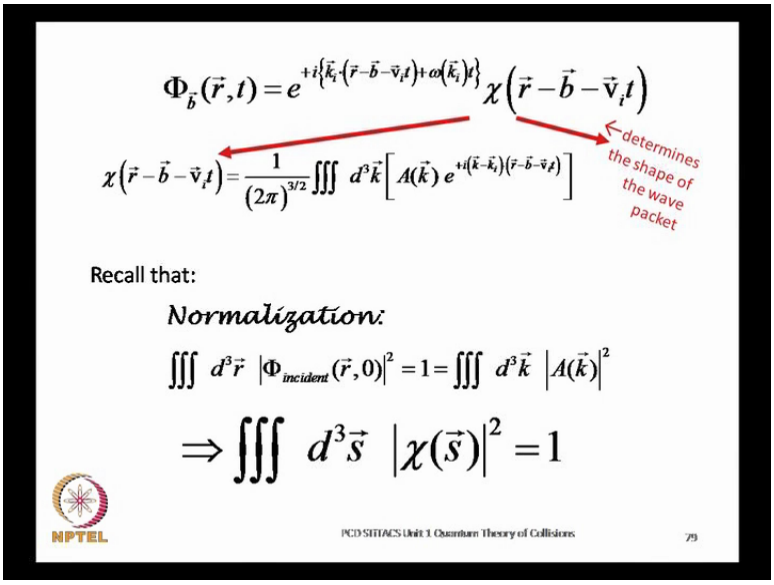

And if you notice that this Chi which is it completely defines the shape of the wave packet. Now you remember that we had an original normalization which we agreed to that we have this normalization. And this normalization is going to be valid for this particular expression out of this, this is just e to the i theta kind of term.

So, the same normalization because what is factored out of the Chi, what multiplies this Chi, is just an e to the i theta kind of term. So obviously you will get the integral of the shape function modular square also equal to 1 okay. So this is a very simple property of the shape function which emerges from this analysis.

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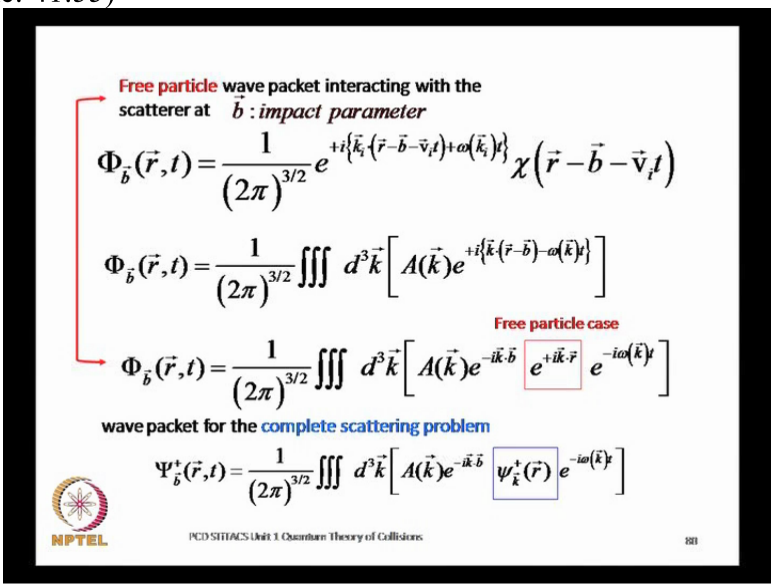

Now this is the free particle wave packet with an impact parameter. Let us write it explicitly we have seen the phase factor to be e to the ik dot r coming from here, e to the - ik dot b coming because of the impact parameter. And this is the omega t factor. This e to the ik dot r is because you are dealing with a free particle case.

And we know how it will get affected if you have scattering right. Because if you now consider the solution to the complete scattering problem now. So, this is the free particle case if you have a complete scattering problem then this factor e to the ik dot r must be replaced by the scattering solution with the outgoing wave boundary condition.

So this e to the ik dot r must be replaced by this solution to the scattering problem with an appropriate outgoing wave boundary condition. But then this is obviously different from the previous case of strict mono energetic beam of incident particles this is a realistic incident beam which consists of a large number of waves which have slightly different momenta corresponding to a slight difference energy spread.

Also the directions could be slightly different and you have got a superposition of all of these different momenta.

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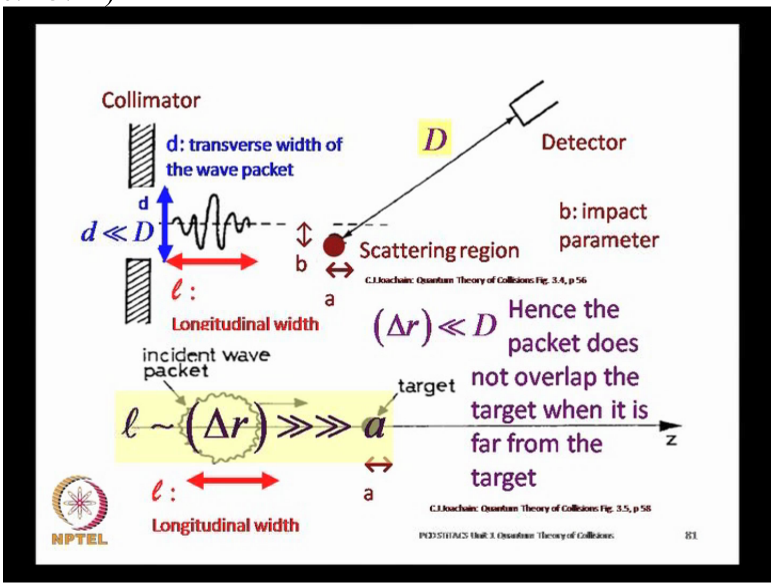

So this is the geometry that you have been considering and the wave packet over this distance okay, it will not overlap with the target when it is far from the target okay. When it reaches the detector it will not have any with the detector. So, this is the geometry you have under consideration.

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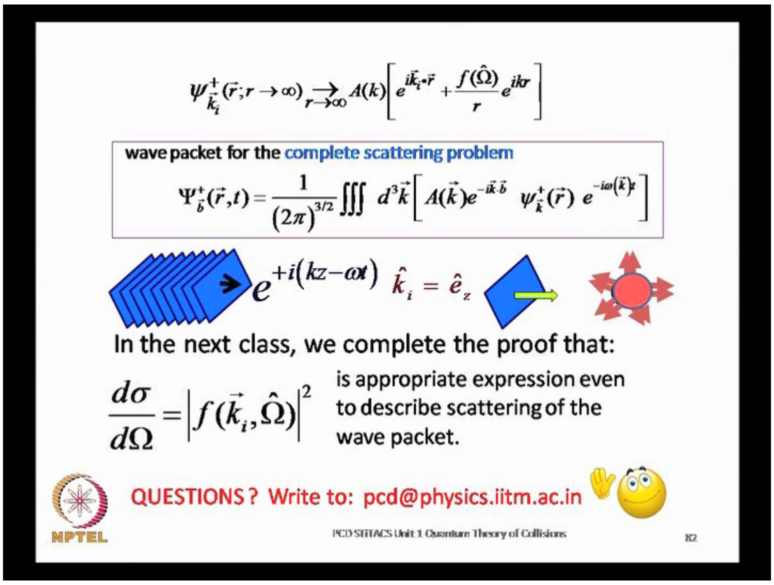

And with this the complete solution to the sketching problem which for pure strict incident waves is given by this outgoing wave boundary condition. Now for the wave packet you have got a similar expression as you had for the free particle incident wave packet with the difference then the term over here which was e to the ik dot r must be replaced by the outgoing wave boundary condition which is this.

Which will not be just the incident wave but the incident wave plus the scattered wave, so we will have to take that into account and since we are out of time I will stop here and in our next class I will complete the proof that with this wave packet which takes into account the impact parameter for the complete scattering solution.

The relationship d sigma by d omega equal to the square of the modulus of the scattering amplitude this is still valid okay. This is the relationship that we set out to prove which we started in our previous class we are almost there. But in the next class we will complete the proof. If there is any question I will be happy to take otherwise goodbye for now.