

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

Lecture 04
 Quantum Theory of collisions- Optical Theorem

(Refer Slide Time: 00:24)

$\vec{j}_{\text{interference}}(\vec{r}) \cdot \hat{e}_r =$ Radial component of the probability current density vector

$$\text{Re} \left\{ \frac{\hbar k}{m} |A(k)|^2 \left[\frac{f(\hat{\Omega}) e^{ikr(1-\cos\theta)}}{r} + \cos\theta \frac{f^*(\hat{\Omega}) e^{-ikr(1-\cos\theta)}}{r} \right] \right\}$$

Incident energy has some spread: \rightarrow spread in magnitude of the wave vector k to $k + \Delta k$

$$\int_k^{k+\Delta k} e^{\pm ik'r(1-\cos\theta)} dk' = \frac{e^{\pm ik'r(1-\cos\theta)}}{\pm ir(1-\cos\theta)} \Big|_k^{k+\Delta k}$$

$$\int_k^{k+\Delta k} e^{\pm ik'r(1-\cos\theta)} dk' = \frac{e^{\pm i(k+\Delta k)r(1-\cos\theta)} - e^{\pm ikr(1-\cos\theta)}}{\pm ir(1-\cos\theta)}$$

numerator $\rightarrow O(1)$
 denominator: $r \rightarrow \infty$

Interference term is of importance only when $\cos\theta \approx 1$
 $\theta \approx 0$

NPTEL IIT Madras STITACS Unit 1 Quantum Theory of Collisions 38

Greetings we will continue our discussion on the optical theorem. We have to establish it which we will today and toward that we considered the probability current density vector which was made up of three terms. The incoming wave, the scattered outgoing wave and then we had the interference term right. And this is the radial component of the current density vector for the interference term.

And we obtain this expression what we realized is that there is a k dependence over here, k dependence is the momentum dependence or energy dependence and even as we imagine that we have a strict mono energetic beam of incident particles. You actually have a little bit of spread in the energy which translates to the momentum in units of \hbar cross going from k to $k + \Delta k$.

The consequence of this is that when you integrate these terms e to the $ikr(1-\cos\theta)$, the other is e to the $-ikr(1-\cos\theta)$. These will need to be integrated over k and when you do that you find that this is a simple integral to evaluate. This is the term that we were discussing toward the end of our previous class and we find that this integral has got these oscillatory terms in the numerator okay.

The numerator is made up of cosine and sine terms and the denominator has got this r and in the asymptotic region as r tends to infinity 1 over r would go to 0. So, you expect this to vanish except when cosine theta = 1 okay. Because then the denominator also goes to 0 and then it can actually blow up right.

So, the interference term is of importance only for small angles, very tiny angles when cosine theta is very nearly equal to 1 or theta is nearly equal to 0. So, this is what we deduced in our previous discussion in the last class that the interference term is of importance only for forward scattering.

So this particular relation which is in this purple rectangular box I have put an additional symbol over here which looks like the Sun okay. This is only to draw your attention to this result this is the radial component of the probability current density vector corresponding to the interference term. And we will come back to this particular expression a little later in the discussion.

So, just as a marker to remember this particular expression I have put this solar symbol over here just to draw your attention to it and we will come back and use this in a later discussion. So, our conclusion is that this interference term is of importance only in the consideration of forward scattering. Otherwise it can be thrown because it consists of oscillatory terms of modulus 1 divided by a denominator which goes to infinity in the asymptotic region. (Refer Slide Time: 03:54)

$$\vec{j}(\vec{r}) \cdot \hat{e}_r = \{ \vec{j}_{\text{incident}}(\vec{r}) + \vec{j}_{\text{outgoing}}(\vec{r}) + \vec{j}_{\text{interference}}(\vec{r}) \} \cdot \hat{e}_r$$

$$dS = r^2 d\Omega \quad \vec{j}(\vec{r}) \cdot r^2 d\Omega \hat{e}_r =$$

$$\{ \vec{j}_{\text{incident}}(\vec{r}) + \vec{j}_{\text{outgoing}}(\vec{r}) + \vec{j}_{\text{interference}}(\vec{r}) \} \cdot r^2 d\Omega \hat{e}_r$$

$$\theta \approx 0$$

$$\iint \vec{j}(\vec{r}) \cdot r^2 d\Omega \hat{e}_r =$$

$$= \iint \{ \vec{j}_{\text{incident}}(\vec{r}) + \vec{j}_{\text{outgoing}}(\vec{r}) + \vec{j}_{\text{interference}}(\vec{r}) \} \cdot r^2 d\Omega \hat{e}_r$$

$$\iint \vec{j}(\vec{r}) \cdot d\vec{S} =$$

$$= \iint \vec{j}_{\text{incident}}(\vec{r}) \cdot d\vec{S} + \iint \vec{j}_{\text{outgoing}}(\vec{r}) \cdot d\vec{S} + \iint \vec{j}_{\text{interference}}(\vec{r}) \cdot d\vec{S} = 0$$

$$\iiint dV \{ \vec{\nabla} \cdot \vec{j}(\vec{r}) \} = \iint \vec{j}(\vec{r}) \cdot d\vec{S} \quad ; \quad \vec{\nabla} \cdot \vec{j}(\vec{r}) = -\frac{\partial \rho}{\partial t}$$

PCD STITACS Unit 1 Quantum Theory of Collisions

Now this is the complete expression for the radial component of the current density vector all the three call contributors are here. The incident beam, the outgoing scatter beam and the interference term, all the three contributors are here. And if you take the flux, so you take the

scalar product of the probability current density vector with a radial elemental surface area which is δs .

Which is like this which is $r^2 \delta \Omega$ times the unit radial outward vector. So, if you take this flux through this elemental area it is the dot product of \mathbf{j} with this δS vector. But \mathbf{j} itself is made up of these three pieces, the \mathbf{j} incident the outgoing and the interference term of which the interference term is going to be important only in the forward scattering region which is θ nearly equal to 0 okay.

So, that is indicated by this reminder here. If you now take a surface integral over a closed surface okay so you have got the scattering experiment taking place in a certain reaction zone. You have got an incident beam and then somewhere far enough you consider a surface which encloses all of this, this whole box okay.

With this whole container where the experiment is taking place and you construct a surface integral of the entire current density vector. So, which is a surface integral of these three contributors to the current density vector over the closed surface, so this is a double integral over a closed surface, there are three terms in the integrand. So you can write it as the sum of three integrals.

One a surface integral of the incident part alone, a surface integral of the outgoing part alone and a surface integral of the interference terminal and this surface integral which is over a closed surface. We know that it is given by the volume integral of the divergence of the current density vector this is just the Gauss's divergence theorem okay. So, by Gauss's divergence theorem we know that the left hand side is nothing.

But the volume integral of the divergence of the current density vector which for stationary state $\nabla \cdot \mathbf{j}$ would vanish. And therefore this whole integral, this surface integral which is equal to the volume integral of the divergence will vanish, it will identically go to zero. The sum of these three terms one, two and three goes to 0 right. Of which the interference term is important only for small angles.

(Refer Slide Time: 06:54)

$$0 = \cancel{\iint \vec{j}_{\text{incident}}(\vec{r}) \cdot d\vec{S}} + \iint \vec{j}_{\text{outgoing}}(\vec{r}) \cdot d\vec{S} + \iint \vec{j}_{\text{interference}}(\vec{r}) \cdot d\vec{S}$$

$$0 = \iint \vec{j}_{\text{outgoing}}(\vec{r}) \cdot d\vec{S} + \iint \vec{j}_{\text{interference}}(\vec{r}) \cdot d\vec{S}$$

$$d\mathcal{D} = \text{scattered outgoing } \vec{j}(\vec{r}) \cdot dS \hat{e}_r \approx |A(k)|^2 \frac{\hbar k}{m} \frac{|f(\hat{\Omega})|^2}{r^2} \hat{e}_r \cdot r^2 d\Omega \hat{e}_r$$

$$\iint \vec{j}_{\text{outgoing}}(\vec{r}) \cdot d\vec{S} = \iint \frac{\hbar k}{m} |A(k)|^2 \frac{|f(\hat{\Omega})|^2}{r^2} \hat{e}_r \cdot r^2 d\Omega \hat{e}_r$$

$$\iint \vec{j}_{\text{outgoing}}(\vec{r}) \cdot d\vec{S} = \frac{\hbar k}{m} |A(k)|^2 \iint |f(\hat{\Omega})|^2 d\Omega = \frac{\hbar k}{m} |A(k)|^2 \sigma_{\text{total}}$$

$$\iint \vec{j}_{\text{interference}}(\vec{r}) \cdot d\vec{S} = \int_{\theta=0}^{\theta=0+\Delta\theta} \sin\theta d\theta \int_{\varphi=0}^{2\pi} d\varphi \vec{j}_{\text{interference}}(\vec{r}) \cdot d\vec{S} \quad \left[\frac{d\sigma}{d\Omega} = |f(\hat{\Omega})|^2 \right]$$

$\theta \approx 0$ $\Delta\theta = ?$ small: $\Delta\theta \neq 0$

NPTEL STITACS Unit 1 Quantum Theory of Collisions 41

So these are the three integrals summed over 20. What about these three terms? Let us take them one by one. So the incident term this is an incident plane wave you have got a closed surface whatever comes in goes out right. So the surface integral will vanish for this term. So, the first term automatically goes to 0, you strike it out.

Now let us, you have 0 on the left hand side equal to the sum of two terms instead of the third term. The third term is already 0 and these two terms, these two surface integrals add up to 0. And now let us consider the scattered part. So, the outgoing scattered part we have evaluated earlier this is $\vec{j} \cdot \delta \hat{e}_r$, where this is the scattered outgoing function.

And we have found that in the asymptotic region it is given by this expression, we have arrived at this result earlier already. So, we will use it and we find that this surface integral, this integrand is over here. So, this surface integral is the integral of this \hbar cross k over m , you have got the modulus of A square then you got f square over r square or r squared delta Ω or.

Now r square is cancelled there is one in the numerator one the denominator the $\hat{e}_r \cdot \hat{e}_r$ will give you unity. And this is your result that the outgoing flux through a closed surface is equal to, this is the scaling \hbar cross k over A square and then you get the surface integral of this f square $d\Omega$. This is the scattering amplitude as you know right or what is the scattering amplitude? The scattering amplitude is nothing but the differential cross section.

So, differential cross section $d\sigma$ by $d\Omega$, which is integrated over all the angles because this is the integration over the solid angle. So, θ will go from 0 to π , ϕ will go from 0 to 2π right. So, all the angles are considered and therefore you will necessarily get from this integration the total cross section.

Because you are integrating $d\sigma$ by $d\Omega$, yes (Question time: 09:38) what sort of the reason we use to relinquish the first term yeah first term exactly the incident term is just incident wave is a plane wave okay. What is the surface integral evaluating, when you evaluate the total flux okay? You are asking basically this is like a divergence right.

So, how much of flux is coming out but whatever is coming in is also going out. It is a pure incident wave as if the target did not exist okay. It is just the pure incident wave, so if you have a plane wave moving from left to right and you have got an interaction region over here but the first term is not even looking at that interaction. It is the contribution to the current density vector coming from the pure incident wave alone.

What goes in the scattered part is in the middle term, what goes in the interference term is in the third term. There are three contributors, the first term is just the incident part it does not even think about, it does not even look at the target. So, what comes in goes out what is the net divergence 0 right.

So, the first term goes to 0 and now you have this second term which is the scattered outgoing wave when you integrate it over the whole surface you find that it gives you the total cross section, total scattering cross section f^2 has got the dimensions of length square which is the same as dimension of σ right. And then you have got this multiplier h cross k over m modulus of A square.

And now we need to consider this interference term in this red loop okay. This is the last piece that we want to consider but this is of course integration over all the angles but we have already discovered that the only angles of importance so far as the interference term is concerned are those small angles in the neighbourhood of $\theta = 0$, because other angles are not going to make any meaningful contribution okay.

So, typically all angles would involve θ going from 0 to π , ϕ going from 0 to 2π but in this case you know that the integration over θ , the polar angle can be restricted to 0 to $0 + \Delta\theta$, where $\Delta\theta$ is a tiny angle, that is the forward scattering okay. So, what is the value of $\Delta\theta$ is it 0, it is certainly not 0, it is small and no matter how small it is, it is not 0 okay.

It is a tiny angle, so it is not important to speak about it in terms of how many degrees or radians it is. It is important to recognize that it is a tiny angle which corresponds to the scattering in the forward direction. It is a tiny angle but a tiny angle it is and it is not zero

okay. So, delta theta is a small angle which is not equal to 0 okay. Just a qualitative analysis actual numbers are not relevant for our discussion.
(Refer Slide Time: 13:39)

$$\begin{aligned}
 0 &= \iint \vec{j}_{\text{outgoing}}(\vec{r}) \cdot d\vec{S} + \iint \vec{j}_{\text{interference}}(\vec{r}) \cdot d\vec{S} && \text{small} \\
 &= \frac{\hbar k}{m} |A(k)|^2 \sigma_{\text{total}} + \iint \vec{j}_{\text{interference}}(\vec{r}) \cdot \hat{e}_r r^2 d\Omega && \Delta\theta \neq 0 \\
 &= \frac{\hbar k}{m} |A(k)|^2 \sigma_{\text{total}} + \int_{\theta=0}^{\theta=0+\Delta\theta} \sin\theta d\theta \int_{\phi=0}^{2\pi} d\phi \vec{j}_{\text{interference}}(\vec{r}) \cdot \hat{e}_r r^2
 \end{aligned}$$

$$\vec{j}_{\text{interference}}(\vec{r}) \cdot \hat{e}_r = \text{Re} \left\{ \frac{\hbar k}{m} |A(k)|^2 \left[\frac{f(\hat{\Omega}) e^{ikr(1-\cos\theta)}}{r} + \cos\theta \frac{f^*(\hat{\Omega}) e^{-ikr(1-\cos\theta)}}{r} \right] \right\}$$

C.J. Joachin: Quantum Theory of Collisions Eq.3.39, p.51

$$0 = \frac{\hbar k}{m} |A(k)|^2 \sigma_{\text{total}} + \int_{\theta=0}^{\theta=0+\Delta\theta} \sin\theta d\theta \text{Re} \left\{ \frac{\hbar k}{m} |A(k)|^2 \left[\frac{f(\hat{\Omega}) e^{ikr(1-\cos\theta)}}{r} + \cos\theta \frac{f^*(\hat{\Omega}) e^{-ikr(1-\cos\theta)}}{r} \right] \right\} r^2$$

NOTE: $A(k)$ does not matter for subsequent analysis

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 42

So, you have this sum of these two surface integrals which goes to 0 of which the first term the scattered outgoing part gives you the total cross section. The interference term is over here and this is to be done for forward scattering for small angles theta going from 0 to 0 + delta theta, sine theta d theta integration over Phi will give you 2pi because of the azimuthal symmetry about the direction of incidence.

And then the integrand over here is the component of the probability current density vector corresponding to the interference term in the radial outward direction right. So this is your integrand and this integrand we have determined earlier. This is the one that I had marked with this sunshine just to remind ourselves that we have this integrand with us. You can just plug it in over here okay, so just plug it in now what do you get, just plug it in.

So, from the first term you have got left hand side is 0, first term is h cross k over m squared of modulus of A times Sigma which is over here h cross k over m modulus A square and the total cross section plus the second integral there is integration over Phi which gives us 2pi over here. So, that is taken care of and now you have just integration over theta over small angles sine theta d theta.

And you have this real part of the system in this beautiful bracket in the sunshine box okay. So, you just plug it in and now let us evaluate this theta integral okay. The Phi integral is already done. It gives you 2pi, it is taken care of over here, you also notice that this is integration over theta but there are these two terms h cross k over m and squared of modulus of A over, in the first term as well as in the second term.

On the left-hand side you have got a 0, so you can strike this out okay. So, you do not have to write it again. It also means that all our subsequent analysis will be independent of the energy dependent normalization A_k is energy dependent normalization right, at that is not going to matter anymore okay.

A is a normalization index k is the momentum in units of \hbar cross. It is related to energy because energy is \hbar cross square k square over $2m$, so this is the energy dependent normalization and it really does not matter in all our subsequent analysis because the term in A vanishes.

(Refer Slide Time: 17:00)

$$0 = \sigma_{total} + 2\pi \int_{\theta=0}^{\theta=0+\Delta\theta} \sin\theta d\theta \operatorname{Re} \left\{ \left[\frac{f(\hat{\Omega}) e^{ikr(1-\cos\theta)}}{r} + \cos\theta \frac{f^*(\hat{\Omega}) e^{-ikr(1-\cos\theta)}}{r} \right] \right\} r^2$$

$$0 = \sigma_{total} + 2\pi \operatorname{Re} \left\{ \begin{aligned} & f(0) r e^{ikr} \int_{\theta=0}^{\theta=0+\Delta\theta} \sin\theta d\theta e^{-ikr \cos\theta} + \\ & f^*(0) r e^{-ikr} \int_{\theta=0}^{\theta=0+\Delta\theta} \sin\theta d\theta e^{+ikr \cos\theta} \end{aligned} \right\}$$

$$\begin{aligned} \cos\theta &= \mu \\ -\sin\theta d\theta &= d\mu \end{aligned}$$

$$0 = \sigma_{total} + 2\pi \operatorname{Re} \left\{ \begin{aligned} & f(0) r e^{ikr} \int_{\mu=\cos\Delta\theta}^{\mu=1} d\mu e^{-ikr \mu} + \\ & f^*(0) r e^{-ikr} \int_{\mu=\cos\Delta\theta}^{\mu=1} d\mu e^{ikr \mu} \end{aligned} \right\}$$

So, I have now written this without the A , there is something else I may have done, know that I believe that is about it. So, you have 0 equal to the first term, now is the total cross section right because the other multipliers has been taken off. The second term which is coming from the interference term is 2π times integration over this angle. In this you have got one over r in these two terms and there is an r square outside.

So, you can take factor out 1 power of r in the numerator okay, this is integration over theta so all r dependent terms can be taken outside the integral. What are the r dependent terms just r to the power 1 because there is an r squared over r in both the terms okay. So, r will come out, what else will come out over here, this is e to the ikr multiplied by e to the ikr cosine theta okay out of which e to the ikr will come out.

From the second integral e to the $-ikr$ will come out but the integration over e to the $+ikr$ cosine theta will remain in the integral because that includes theta dependence right. What else comes out, now this is sketching over a very tiny small angle in the neighbourhood of

theta = 0 and the scattering amplitudes you expect them to be very slowly varying functions of the angles it will not very change very much in that tiny cone okay.

You understand what I mean by a cone because you have got an incidence direction and from here you have a cone which is diverging out okay. You get the picture or shall I draw it on the board, maybe I will draw it on the board, say what a scattering center here and you have got these plane waves come over here this is your z-axis. So, all angles are measured with respect to this axis and this is your theta.

And what comes out in this cone is scattering in the forward direction right that is the only thing that matters, theta actually goes the polar angle will go from 0 to pi, but the only region of interest is from 0 to 0 + delta theta where delta theta is a very small angle. So, it is only the scattering in this forward direction which is of importance.

And in this small tiny angle this is the little tiny cone, the scattering amplitude which is a function of theta, f of omega which is the function of theta is not going to change very much in that very tiny angle. So, f of omega which is in the integrand can also be taken out. So, you have got f at theta = 0 which is the forward scattering amplitude okay.

This r is coming from the r square over r and then e to the ikr and what is being integrated is e to the - ikr cosine theta from the first term. And from the second term you will have this e to the - ikr + 1 -cos theta right. So what does it give you, so if you put cosine theta equal to mu, just a simple substitution, if you do this simple substitution you get total cross section over here, 2pi over here and then you have this fo r e ot the ikr.
(Refer Slide Time: 21:42)

$$\sigma_0 = \sigma_{total} + 2\pi \operatorname{Re} \left\{ f(0) r e^{ikr} \int_{\mu=\cos\Delta\theta}^{\mu=1} d\mu e^{-ikr\mu} + f^*(0) r e^{-ikr} \int_{\mu=\cos\Delta\theta}^{\mu=1} d\mu e^{ikr\mu} \right\}$$

$$\sigma_0 = \sigma_{total} + 2\pi \operatorname{Re} \left\{ f(0) r e^{ikr} \left[\frac{e^{-ikr\mu}}{-ikr} \right]_{\mu=\cos\Delta\theta}^{\mu=1} + f^*(0) r e^{-ikr} \left[\frac{e^{ikr\mu}}{ikr} \right]_{\mu=\cos\Delta\theta}^{\mu=1} \right\}$$

$$\sigma_0 = \sigma_{total} + 2\pi \operatorname{Re} \left\{ \begin{aligned} & f(0) \dagger e^{ikr} \left[\frac{e^{-ikr} - e^{-ikr\cos\Delta\theta}}{-ikr} \right] + \\ & f^*(0) \dagger e^{-ikr} \left[\frac{e^{ikr} - e^{ikr\cos\Delta\theta}}{ikr} \right] \end{aligned} \right\}$$

$$\sigma_0 = \sigma_{total} + 2\pi \operatorname{Re} \left\{ \begin{aligned} & f(0) \left[\frac{1}{-ik} - \frac{e^{ikr(1-\cos\Delta\theta)}}{-ik} \right] + \\ & f^*(0) \left[\frac{1}{ik} - \frac{e^{-ikr(1-\cos\Delta\theta)}}{ik} \right] \end{aligned} \right\}$$

NPTEL

PCD STITACS Unit 1 Quantum Theory of Collisions 44

And then you have the integration of e to the -ikr over -ikr, you put the limits. Now mind you, this is sine theta d theta right, so the limits from 0 to 0 + delta theta because of the minus sign will go from mu equal to cos delta theta to mu = 1 okay. So, these sign limits; this is because of the change in sign, so what you get, you have got this complete expression now.

You have total cross section here 2pi times, the real part of these terms. You have got e to the -ikr, these are actually two terms with -1 -ikr in the denominator and the difference between -ikr, which is the value at mu = 1 and e to the -ikr and the value of mu = cos delta theta. So, these are the two terms coming from here and these are the corresponding two terms coming from here right.

Now you notice that this r cancels this r, you also notice that this r cancels this r. So, there is a lot of simplification, in fact all this is going to lead us to a very simple tiny compact beautiful result. So, the r cancels then you multiply this e to the ikr with this e to the -ikr that gives you 1. So, you get 1 over -ik from the first term. So, you just do this little simplification and you have a very simple set of analysis coming out.

And then here you have got e to the ikr multiplying each of the -ikr cos delta theta. So, that will give you e to the ikr times 1 -cos delta theta okay right. So this is what you get from this pair of terms and you have a similar expression from the second pair of terms. So, the algebra of the mathematics is rather straightforward.

(Refer Slide Time: 24:28)

$$0 = \sigma_{total} + 2\pi \operatorname{Re} \left\{ \begin{aligned} & f(0) \left[\frac{1}{-ik} - \frac{e^{ikr(1-\cos\Delta\theta)}}{-ik} \right] + \\ & f^*(0) \left[\frac{1}{ik} - \frac{e^{-ikr(1-\cos\Delta\theta)}}{ik} \right] \end{aligned} \right\}$$

$$\int_k^{k+\Delta k} e^{\pm ik'r(1-\cos\Delta\theta)} dk' = \frac{e^{\pm i(k+\Delta k)r(1-\cos\Delta\theta)} - e^{\pm ikr(1-\cos\Delta\theta)}}{\pm ir(1-\cos\Delta\theta)}$$

$\Delta\theta \neq 0$ however small

$$0 = \sigma_{total} + 2\pi \operatorname{Re} \left\{ \begin{aligned} & f(0) \left[\frac{i}{k} + \text{oscillatory terms} \right] + \\ & f^*(0) \left[\frac{-i}{k} + \text{oscillatory terms} \right] \end{aligned} \right\}$$

$\rightarrow 0$ as $r \rightarrow \infty$

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 45

These are the two terms; now, here when you integrate over k, when you consider a wave packet. When you consider the energy spread okay, we have considered this integral but this time we know that we are considering a tiny angle delta theta which is not zero okay. So, there is an asymptotic region so as r tends to infinity.

If you look at these two terms the numerator consists of oscillatory cosine and sine terms of modulus 1 and the denominator has r going to infinity. So these oscillatory terms will vanish because no longer is $\Delta\theta$ equal to 0. It is a tiny angle, no matter what how small, no matter how small it is because you keep going far enough. And asymptotic, asymptotic region is r tending to infinity there is something very beautiful infinite about infinity.

That no matter how far in distance, you consider, you always consider a distance beyond right. And so far as our experimental setup is concerned, it is a very practical situation because the scattering takes place in a certain zone, scattering region okay. Outside this region the scattering potential has practically no influence and the detectors are kept far away from the reaction zone.

So, far that the scattering potential has got no influence at the detector right, so for all practical purposes this is infinity in our context, it is a very meaningful infinity okay. Because infinity does not really mean that you have to go billions of kilometers and beyond the edge of the universe, only cosmic could do that right. That is not infinity it is far away sufficiently far, so that the scattering potential has no influence over there.

And the scattering potentials are physical interactions they all die as you go away from them right. So this result has got terms coming from this region in the small cone $\Delta\theta$ no matter how small it is over here for this consideration, it is not zero. What it means, that the total cross section coming from the first term is here. From the interference term you have 2π and then f_0 this is 1 over $-ik$, which is the same as $+i$ over k okay.

I have taken the i to the numerator likewise I have taken this i to the numerator, so it becomes $-i$ over k . And then you I have got oscillatory terms which vanish as r tends to infinity so you can throw them out. And now you have only this f_0 i over k + f^* , which is a complex conjugate of the forward scattering amplitude times $-i$ over k .
(Refer Slide Time: 28:13)

$$0 = \sigma_{total} + 2\pi \operatorname{Re} \left\{ f(0) \left[\frac{i}{k} \right] + f^*(0) \left[\frac{-i}{k} \right] \right\}$$
The total scattering x-sec is equal to $4\pi/k$ times the imaginary part of the forward (complex) scattering amplitude

$$0 = \sigma_{total} + 2\pi \operatorname{Re} \left\{ 2 \operatorname{Re} \left(f(0) \left[\frac{i}{k} \right] \right) \right\}$$

$$0 = \sigma_{total} + \frac{4\pi}{k} \operatorname{Re} \left\{ \operatorname{Re} (i \times f(0)) \right\}$$

$$0 = \sigma_{total} + \frac{4\pi}{k} [-\operatorname{Im} f(0)]$$

$$\sigma_{total} = \frac{4\pi}{k} [\operatorname{Im} f(0)]$$

OPTICAL THEOREM
 Bohr-Peierls-Placzek relation

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 46

So that is what you got $f(0) \times i/k + f^*(0) \times -i/k$. And you already notice that these two are complex conjugates of each other. So it is like taking a number $a + ib$ and adding to it $a - ib$, what do you get twice of a , twice the real part right. So this is the twice the real part of the first term which is $f(0) \times i/k$ right. Twice the real part of the complex number okay, now we have to find this, how do you hit that $f(0) \times i/k$, f is a complex scattering amplitude okay.

So here this 2 into this 2 will give you 4, so you get 4π there is a k in the denominator, so you get $4\pi/k$. Now you get the real part of this, real part of i times the forward scattering amplitude okay, $i \times f(0)$, $f(0)$ is some complex number, let us say it is $a + ib$, $i \times f(0)$ will be $ia - b$ right.

So, the real part of this is $-b$ okay. So, this is minus the imaginary part of the forward scattering amplitude which is a real number okay. The complex number consists of two real numbers and the imaginary part is as real as the real part right. So you get minus imaginary part of the forward scattering amplitude.

So, let us plug it in over here, in this relation and you get 0 equal to $\sigma_{total} + 4\pi/k$ times minus imaginary part of the complex forward scattering amplitude. So, this gives us an expression for the total cross section, what is it? It is equal to $4\pi/k$ times the imaginary part of the complex forward scattering amplitude. This is the optical theorem; this is called as optical theorem.

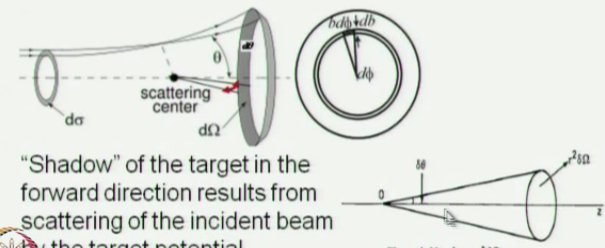
It is also known as Bohr Peierls Placzek, so this is also called as Bohr relation okay. Bohr a power let us say okay. So, this is the optical theorem, it tells us that the total cross section is equal to $4\pi/k$ times the imaginary part of the forward scattering amplitude.

(Refer Slide Time: 31:08)

$$\sigma_{total} = \frac{4\pi}{k} [\text{Im } f(0)]$$
OPTICAL THEOREM
 Bohr-Peierls-Placzek relation

ORIGINS:

$$\iiint dV \{ \vec{\nabla} \cdot \vec{j}(\vec{r}) \} = \iint \vec{j}(\vec{r}) \cdot d\vec{S} ; \vec{\nabla} \cdot \vec{j}(\vec{r}) = -\frac{\partial \rho}{\partial t}$$



“Shadow” of the target in the forward direction results from scattering of the incident beam by the target potential.

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions C.J. Joachain: Quantum Theory of Collisions Fig. 3.3, p.53 47

Its origin is in the equation of continuity. So it is essentially statement of conservation of flux okay. You are not trading particles you are not destroying particles. So, it has its energy in conservation of flux, it is similar to an optical effect which is why it is called as an optical theorem because whenever light is incident it meets an obstacle which scatters it in various directions.

And there is a diminished intensity behind it right. So, it is a certain shadow effect and this is what is happening this is the cone, I was referring to. That, this is the tiny small angle delta theta okay and you have this scattering, the scattering is not necessarily a physical encounter between the projectile and the target because the encounter is through a physical interaction not a bodily encounter as happens in a crowd okay.

But this is a physical interaction, so that incident particles are deflected away and this is the scattering cross section that we get. We find that this result is completely independent of the energy dependent normalization because it fell off from our analysis already.

(Refer Slide Time: 32:31)

Outgoing wave boundary condition $\Psi_{\vec{k}_i}^+(\vec{r}; r \rightarrow \infty) \xrightarrow{r \rightarrow \infty} A(\vec{k}_i) \left[e^{i\vec{k}_i \cdot \vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr} \right]$


$C_l = e^{i\delta_l(k)}$ We have employed this boundary condition, inclusive of an l -dependent normalization.

describes 'collisions'

$A(\vec{k})$: energy dependent normalization of the incident wave that scales the scattered part as well.

OPTICAL THEOREM: independent of $A(\vec{k})$

scattering x-sec per unit solid angle differential x-sec $\frac{d\sigma}{d\Omega} = |f(\hat{\Omega})|^2$ This definition is independent of the normalization

 PCD STITACS Unit 1 Quantum Theory of Collisions 48

What we did make use of their outgoing wave boundary conditions? We used the collision boundary conditions in this particular analysis as opposed to the ingoing wave photoionization boundary conditions. We concluded that the optical theorem is independent of the energy dependent normalization.

And we also in the course of our derivation we recognized that the differential cross section is nothing but the square of the modulus of the scattering amplitude and this definition again is independent of the normalization. So, these are the main features of our analysis that we have got so far.


(Refer Slide Time: 33:34)

$\Psi_{\vec{k}_i}^+(\vec{r}; r \rightarrow \infty) \xrightarrow{r \rightarrow \infty} A(\vec{k}_i) \left[e^{i\vec{k}_i \cdot \vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr} \right]$

scattering x-sec per unit solid angle differential x-sec $\frac{d\sigma}{d\Omega} = |f(\hat{\Omega})|^2$ This definition is independent of the normalization

$\Psi_{\text{tot}}^+(\vec{r}, t) \Big|_{r \rightarrow \infty} \rightarrow \frac{1}{(2\pi)^{3/2}} A(\vec{k}) \left[e^{+i(\vec{k} \cdot \vec{r} - \omega t)} + \frac{e^{+i(kr - \omega t)}}{r} \left\{ \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [e^{2i\delta_l(k)} - 1] P_l(\cos \theta) \right\} \right]$

We employed mono-energetic incident beam → idealization

 PCD STITACS Unit 1 Quantum Theory of Collisions 49

What it gives us is the total cross total solution to the scattering problem. This is the time independent part together with the time dependent part you get an incident plane wave and a scattered spherical outgoing wave. And this is the Faxen Holtzmark's resolution of the

scattering amplitude the partial wave decomposition. What we have used mostly except for putting in some details our primary results are for a mono energetic plane wave.

This is our incident beam which consists of an energy which is $\hbar^2 k^2 / 2m$ and this is the momentum vector \vec{k} a single energy is what we have considered mostly right. You have considered the energy spread to deal with certain detailed aspects of some mathematical terms but our basic formalism has been geared to the consideration of a mono energetic incident beam. Now this is a rather ideal situation we know okay. (Refer Slide Time: 34:44)

mono-energetic / idealization

$$\psi_{Tot}^*(\vec{r}, t) \Big|_{r \rightarrow \infty} = \frac{1}{(2\pi)^{3/2}} A(\vec{k}) \left[e^{+i(\vec{k}\vec{r} - \omega t)} + \frac{e^{+i(\vec{k}r - \omega t)}}{r} \left\{ \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [e^{2i\delta_l(k)} - 1] P_l(\cos\theta) \right\} \right]$$

$$\frac{d\sigma}{d\Omega} = |f(\vec{k}_i, \hat{\Omega})|^2 \rightarrow \text{monoenergetic idealization of incident beam properties}$$

incident beam properties

$$\Phi_{incident}(\vec{r}, t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i(\vec{k}\vec{r} - \omega t)} \right]$$

$$= \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i(\vec{k}\vec{r} - \omega(k)t)} \right]$$

Realistic incident wave packet

Does the expression for the differential scattering cross-section, which is $\frac{d\sigma}{d\Omega} = |f(\vec{k}_i, \hat{\Omega})|^2$ hold good even to describe scattering of the wave packet?

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 50

This is not always what we are going to have we will typically have a result which will have to include the energy spread. And what we have found is that this relation $d\sigma/d\Omega = |f|^2$ is correct for a mono energetic idealization of the incident beam particles.

But a typical incident wave will be a wave packet in which you will carry out integration over the momentum okay. There will be several wavelengths which are present or several frequencies if like, several energies. And a realistic incident wave packet will have an expression of this kind right.

It will be a superposition of plane waves that each term is a plane wave $e^{i(\vec{k}\vec{r} - \omega t)}$ is a plane wave right. Each is scaled by an energy-dependent normalization and when you add all of these terms that is when you get an incident wave that is an incident wave packet rather than a pure plane wave.

So, this incident wave packet is what we must consider and the question we are now going to ask is whether or not this expression $d\sigma/d\Omega = |f|^2$ is correct for the scattering of a wave packet.

is this valid even in the case of a realistic incident wave packet which is given by the superposition of plane waves.

And we will find that in fact it is, that it is correct this equation, relationship survives even the consideration of an incident wave packet so that is what we are going to discuss now. Is this part clear; very good.
(Refer Slide Time: 36:55)

Slide 51 content:

$$\Phi_{\text{incident}}(\vec{r}, t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i(\vec{k}\vec{r} - \omega t)} \right]$$

$$= \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i(\vec{k}\vec{r} - \omega(k)t)} \right]$$

Realistic incident wave packet

$A(\vec{k})$ can be determined if the wave-packet is known at $t=0$

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 51

So, let us now consider a realistic incident wave packet and this is the energy dependent normalization you can always get it if you know what the wave packet is at the initial time t equal to zero okay.
(Refer Slide Time: 37:08)

Slide 52 content:

$$\Phi_{\text{incident}}(\vec{r}, t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i(\vec{k}\vec{r} - \omega t)} \right]$$

$$= \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i(\vec{k}\vec{r} - \omega(k)t)} \right]$$

Realistic incident wave packet

$$\omega(k) = \frac{E(k)}{\hbar} = \frac{\hbar^2 k^2}{2m} \frac{1}{\hbar} = \frac{\hbar k^2}{2m}$$

Group velocity
Particle velocity $\left[\frac{d\omega(k)}{dk} \right]_{k_i} = \frac{\hbar k_i}{m} = \mathbf{V}_i$

$$\left[\vec{\nabla}_k \omega(\vec{k}) \right]_{\vec{k}_i} = \vec{v}_i$$

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 52

So, let us consider a realistic incident wave packet. In this there will be an energy momentum relationship okay. Let us consider that this is the energy momentum relationship so this omega is not independent of k right. In fact it is a quadratic function of k because omega is e

over \hbar cross, e is \hbar cross square k squared over $2m$ this divided by \hbar cross will give you \hbar cross over $2m$ times k square.

So, ω is a function of k right like you have an a dispersion relation. So, you have got a k dependent frequency okay, k dependent ω and you can then determine the group velocity which is given by the derivative of the frequency with respect to k . What is this derivative, derivative of \hbar cross k square by $2m$ with respect to k , so you get the velocity.

So, this is the particle velocity or the group velocity okay. Now you can consider a vectorial; you know generalization of this relationship. So it is not just the derivative with respect to k but k is a vector. So, you must take the gradient of ω okay and this gradient will give you the velocity vector in one dimension.

If there is only one direction you have just V_i , the scalar right the magnitude of the velocity but when you have vectors you take the gradient of the k dependent ω that gives you the velocity vector so this is a well known result.

(Refer Slide Time: 39:18)

$$\Phi_{\text{incident}}(\vec{r}, t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i(\vec{k}\vec{r} - \omega(\vec{k})t)} \right] \quad A(\vec{k}) \text{ can be}$$
Eq. 3.57 / p.55 / Joachain's Quantum Collision Theory
 Realistic incident wave packet determined if the wave-packet

$$\Phi_{\text{incident}}(\vec{r}, 0) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i\vec{k}\vec{r}} \right] \quad \text{is known at } t=0$$

$$A(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{r} \left[\Phi_{\text{incident}}(\vec{r}, 0) e^{-i\vec{k}\vec{r}} \right] \quad \text{wave-function in the momentum (rather, 'wave-vector') space known at } t=0$$
Eq. 3.59 / p.55 / Joachain's Quantum Collision Theory

Each individual wave $\frac{1}{(2\pi)^{3/2}} A(\vec{k}) e^{+i(\vec{k}\vec{r} - \omega(\vec{k})t)}$

travels at the phase velocity

$$v_{\text{phase}} = \frac{\omega(k)}{k} = \frac{E(k)/\hbar}{k} = \frac{(\hbar k)^2 / 2m}{\hbar k} = \frac{\hbar k}{2m}$$
Eq. 3.60 / p.55 / Joachain's Quantum Collision Theory

Phase velocity is half the group velocity

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 53

Let us determine A from $t = 0$ because at $t = 0$ the ωt term will vanish okay, e to the i ωt , will be e to the 0 which is 1 , so you get for $t = 0$, which is what I have written here this is the argument $t = 0$ and there is no time dependent term on the right side in the integrand. And from this relation if you just do a Fourier inward of this you get A as this integral which is nothing but the wave function in the momentum space right.

So this is just the wave function in the momentum space and each individual wave there are so many individual ways for different values of k right. Each travels at a phase velocity but the wave packet travels at the group velocity. So, the phase velocity for each component is

given by ω/k which is $h \times \text{square } h \times k$ over $2m$. As you can see easily from this relation, what it means is that the phase velocity is halved the group velocity in this case right, this is a well known result.
(Refer Slide Time: 40:45)

$$\Phi_{incident}(\vec{r}, t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{i(\vec{k}\cdot\vec{r} - \omega(\vec{k})t)} \right]$$

Realistic incident wave packet at $t=0$:

$$\Phi_{incident}(\vec{r}, 0) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{i\vec{k}\cdot\vec{r}} \right] \quad \leftarrow \Delta k \ll |\vec{k}_i|$$

narrow spread

$$A(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{r} \left[\Phi_{incident}(\vec{r}, 0) e^{-i\vec{k}\cdot\vec{r}} \right]$$

'spread/packed' in the region

$\Delta r = \frac{1}{\Delta k}$

Normalization:

$$\iiint d^3\vec{r} |\Phi_{incident}(\vec{r}, 0)|^2 = 1 = \iiint d^3\vec{k} |A(\vec{k})|^2 \quad \text{Let } A(\vec{k}) = |A(\vec{k})| e^{i\alpha(\vec{k})}$$

$$\Phi_{incident}(\vec{r}, t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[|A(\vec{k})| e^{i\alpha(\vec{k})} e^{i\vec{k}\cdot\vec{r}} e^{-i\omega(\vec{k})t} \right]$$

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 54

Typically there is a narrow spread it is not that k really goes from minus infinity to plus infinity or something like that there is a some sort of a narrow spread. Because it is a reasonably mono energetic beam it is not strictly fully purely a mono energetic it is a reasonably energetic beam.

And it is a Fourier transform will also be there for confined to some sort of a location Δr which will depend on the inverse of the spread in momentum okay. So this is just the position momentum complementarity. You consider a normalization in the real space and the momentum space. They are Fourier transforms of each other.

So, they must both be normalized appropriately, A is some complex scaling factor. So, let us say that this is its modulus part and α is the phase part, so you can write any complex number as $Rho e^{i\theta}$, where Rho is the magnitude of the complex number. And the phase over here is α which depends on k .

So, the incident wave packet is $1 / (2\pi)^{3/2}$ this integral over all the momenta of this term A of k is now modulus of A times this phase angle which is $e^{i\alpha k}$. And then you have got these two terms which is $e^{i\vec{k}\cdot\vec{r}}$ and $e^{-i\omega t}$, where ω depends on k .

(Refer Slide Time: 42:34)

$$\Phi_{\text{incident}}(\vec{r}, t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i(\vec{k}\cdot\vec{r} - \omega(\vec{k})t)} \right]$$

Realistic incident wave packet at $t=0$:

Let $A(\vec{k}) = |A(\vec{k})| e^{i\alpha(\vec{k})}$

$$\Phi_{\text{incident}}(\vec{r}, t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[|A(\vec{k})| e^{i\alpha(\vec{k})} e^{+i\vec{k}\cdot\vec{r}} e^{-i\omega(\vec{k})t} \right]$$

$$\Phi_{\text{incident}}(\vec{r}, t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} |A(\vec{k})| e^{i\beta(\vec{k})}$$

$$\beta(\vec{k}) = \vec{k}\cdot\vec{r} - \omega(\vec{k})t + \alpha(\vec{k})$$

NPTEL Eq 3.55, 3.56 / p56 / Joachain's Quantum Collision Theory
PCD STITACS Unit 1 Quantum Theory of Collisions 55

So, what is under consideration is a realistic incident wave packet this is our decomposition into the real part in the phase part the modulus of the complex number. And having considered this we write the incident wave packet as this modulus times e to the i beta where this beta phase is the sum of these three angles alpha + k dot r. This is k dot r, this is alpha and - omega t. So these are the three angles which sum up which together gives us the phase which is what we call as beta.
(Refer Slide Time: 43:28)

$$\Phi_{\text{incident}}(\vec{r}, t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[|A(\vec{k})| e^{i\beta(\vec{k})} \right] \quad \beta(\vec{k}) = \vec{k}\cdot\vec{r} - \omega(\vec{k})t + \alpha(\vec{k})$$

Under what conditions is $|\Phi_{\text{incident}}(\vec{r}, t)|$ the largest?

$e^{i\beta(\vec{k})} \rightarrow$ oscillates in response to \vec{k} since $\beta = \beta(\vec{k})$
oscillating parts cancel each other's contributions to $\Phi_{\text{incident}}(\vec{r}, t)$

For $|\Phi_{\text{incident}}(\vec{r}, t)|$ to be large, these oscillations must not happen
 β must not vary very much with respect to \vec{k}

The required condition is:

$$\left[\vec{\nabla}_{\vec{k}} \beta(\vec{k}) \right]_{\vec{k}=\vec{k}_i} = 0$$

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 56

So, this is your beta. Now let us ask this question when is the modulus of the incident wave, the largest. It should have with some significant value right if it is zero you have nothing to scatter right. And what is being added integration is just the limit of a sum you are adding terms in which you have got an oscillatory part e to the i beta k. In which the oscillations will change with k, the phase changes with k, the integration is because of the change in k. The phase is k dependent and if the dependence on k is very strong there will be oscillations and all of those terms will cancel each other okay. So, for the

incident wave packet to survive the condition is the recognition of the fact that the oscillations are dying because of the k dependence of the angle beta.

And therefore for the oscillations not to kill the incident wave packet, our requirement must be that these oscillations must not take place. When will this not happen, when beta is not a function of k or at least it is not a strong function of k, it is a weak function of k, it is nearly independent of k, if d beta by dk goes to 0 right.

So, our condition is that beta must not change very much with respect to k, that is the condition that must be satisfied which means that the gradient of beta with respect to k at this initial k vector, this k vector of the incident beam, this gradient vanishes, this is our condition. (Refer Slide Time: 45:58)

condition for $\left[\vec{\nabla}_k \beta(k) \right]_{\vec{k}=\vec{k}_i} = 0$ $\beta(\vec{k}) = \vec{k} \cdot \vec{r} - \omega(\vec{k})t + \alpha(\vec{k})$
 $= kz - \omega(\vec{k})t + \alpha(\vec{k})$
Eq. 3.65, 3.66 / p56 / Joachain's Quantum Collision Theory

$|\Phi_{incident}(\vec{r}, t)|$ to be the largest

1-dimensional case \rightarrow $0 = \left. \frac{d\beta(k)}{dk} \right|_{k_i} = z - \left[\left. \frac{d\omega(k)}{dk} \right]_{k_i} t + \left[\left. \frac{d\alpha(k)}{dk} \right]_{k_i}$
 i.e. $z = \left[\left. \frac{d\omega(k)}{dk} \right]_{k_i} t - \left[\left. \frac{d\alpha(k)}{dk} \right]_{k_i}$

3-dimensional case \rightarrow $\vec{r}(t) = \left[\left. \vec{\nabla}_k \omega(\vec{k}) \right]_{\vec{k}_i} t - \left[\left. \vec{\nabla}_k \alpha(\vec{k}) \right]_{\vec{k}_i}$

Time origin: t_0 $\vec{r}(t) = \vec{v}_i (t - t_0) + \vec{r}_0$
 \rightarrow since $\vec{v}_i = \left[\left. \vec{\nabla}_k \omega(\vec{k}) \right]_{\vec{k}_i}$ & $\vec{r}_0 = - \left[\left. \vec{\nabla}_k \alpha(\vec{k}) \right]_{\vec{k}_i}$

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 57

So, for this incident wave packet to be the largest the gradient of beta must vanish, beta is the sum of these three terms k dot r is kz. Because we have chosen z to be r cos theta okay, that is the direction of the incident beam that we have chosen. So, beta must be equal to kz - omega kt + alpha its derivative with respect to k must vanish.

So 0 = db term dk at k corresponding to the incident k. So, d beta by dk from the first term gives you z, from the second term you get d omega by dk.

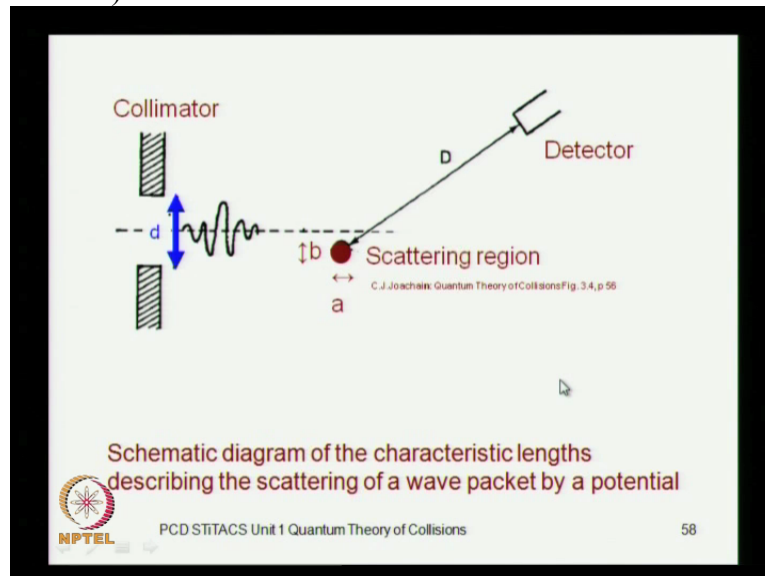
And from the third term multiplied by t of course, from the third term you get d alpha by dt this is a one dimensional result. In three dimensions you will have the position vector r equal to the gradient of omega t - the gradient of alpha okay. It is a straightforward generalization to three dimensions.

Now this minus gradient of alpha, of course each of these term is a distance vector left hand side is just the distance vector, it is a position vector. So, this is the distance vector which we

call as $\mathbf{r}_0 - \nabla \alpha$ is what is called as \mathbf{r}_0 gradient of α is the velocity which we have just seen few minutes ago right.

So, gradient of α gives you velocity and if you have the time origin at t_0 you get a function, of the position vector as a function of time which is velocity times the time difference from 0, from the initial time which is $t - t_0$. And then there is a new vector \mathbf{r}_0 which is defined in terms of the gradient of α .

(Refer Slide Time: 47:59)



So this is the kind of schematic diagram under consideration that you have got the source of an incident beam, you have got a collimator, you have got a little bit of transfer spread, a little bit of longitudinal spread of the wave packet and then you have got scattering and then these terms arrive at a certain impact parameter distance okay.

And then you consider the detection in a region which is sufficiently far so that is the kind of experimental setup that you have and you have these distance scales that the wave packet is confined over a certain region which goes as the inverse of the spread in the momentum in units of \hbar cross right. So that is what you have got.


(Refer Slide Time: 48:56)

$$\Phi_{\text{incident}}(\vec{r}, t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{i\beta(\vec{k})} \right] \quad \beta(\vec{k}) = \vec{k} \cdot \vec{r} - \omega(\vec{k})t + \alpha(\vec{k})$$


$$\Phi_{\text{incident}}(\vec{r}, t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{i\{\vec{k} \cdot \vec{r} - \omega(\vec{k})t + \alpha(\vec{k})\}} \right]$$

$$\omega(\vec{k}) = \omega(\vec{k}_i) + \left[\vec{\nabla}_k \omega(\vec{k}) \right]_{\vec{k}_i} \cdot (\vec{k} - \vec{k}_i) + \dots$$

$$= \omega(\vec{k}_i) + \vec{v}_i \cdot (\vec{k} - \vec{k}_i) + \dots$$

$$= \omega(\vec{k}_i) + \vec{v}_i \cdot \vec{k} - \vec{v}_i \cdot \vec{k}_i + \dots$$


QUESTIONS? Write to: pcd@physics.iitm.ac.in



PCDSIITACS Unit 1 Quantum Theory of Collisions

59

And let us have a look at this k dependence of this omega. So, let us write this as an expansion. So, k dependence of omega you have got expanding it about a certain direction of incidence corresponding to one particular momentum value which is k_i . So, this is the first term this is the leading term then you have got the gradient times the difference and then you have got additional terms which we will ignore.

But then we will also ask later under what conditions you can ignore those terms okay. So, that question we will take up later, for the time being we will just consider this and I guess I will stop here for today and we will take up the discussion from this point in the next class. Questions, (Question time: 50:07) is dependent on k beta is beta of K correct it is very slowly depending on k yeah, is it realistic or non realistic.

That is the only time when the wave packet exists otherwise the oscillatory parts cancel each other and you do not have any incident wave. So in all scattering experiments when you have an incident beam and there is a little bit of spread then automatically this takes care. (Not audible: 50:56) yeah it does not matter because if the wave packet is spread out over a width like this okay.

There is a transverse width and there is a longitudinal width okay. They are typically of the same size just an order of magnitude and the size is goes as one over the spread in the momentum $1/\Delta k$ and for wave packets of this kind you have the beta to go by this. So, essentially what is happening is that the group velocity and the gradient of this alpha term they adjust to each other.

So, that $d\beta/dk$ goes to 0, which means that the sum of these three terms goes to zero. It means that the condition that the wave packet does not disappear or does not vanish because

of the oscillatory terms is automatically generated by the group velocity yeah. (Question time: 52:56) It does not mean that it is varying very slowly with respect to k , does not mean; well slow enough, slow enough for this approximation to hold.

It does not mean that beta does not depend on k at all but its dependence is mild okay. If you plot beta as a function of k , if you have large oscillations ups and downs it means that it is changing rapidly with k . If it is flat it means that it does not change with k at all, dy by dx is 0, if y is parallel to the x -axis right.

So, beta need not be exactly parallel, but if it is nearly parallel if it has got small ripples that is good enough. If it has these large oscillations then it will die out okay, smaller oscillations does not matter okay. So thank you very much.