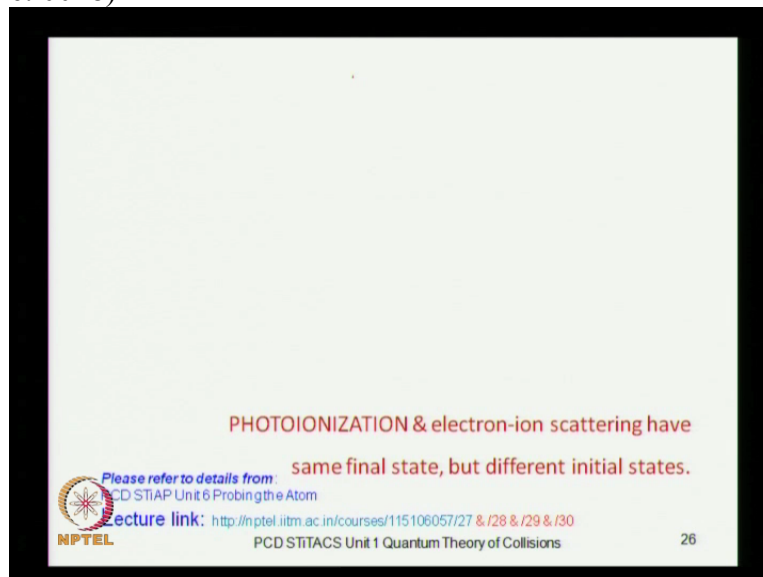


Select/Special Topics in 'Theory of Atomic Collisions and Spectroscopy'
Prof. P.C. Deshmukh
Department of Physics
Indian Institute of Technology-Madras

Lecture 03
Quantum Theory of collisions- Optical Theorem

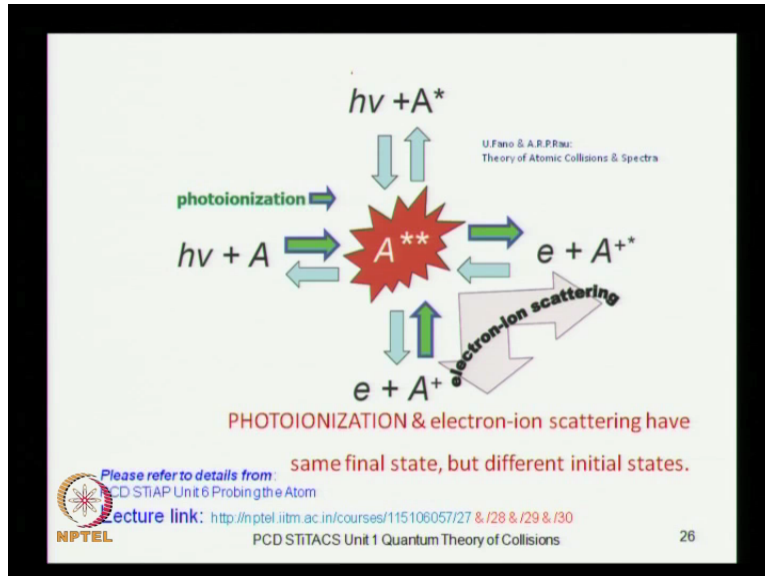
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Greetings, will discuss the optical theorem today, this is a very well-known theorem in collision physics. Anybody and everybody who does collision physics knows this theorem and let me remind you that in the previous course that we did which is the special select topics in atomic physics. We discussed photoionization and electron ion scattering as two aspects of the same quantum physics.

That these two phenomena are intimately connected to each other and a detailed discussion on this is available in unit 6 of the previous course and these lecture number 27, 28, 29 and 30 at this link summarize the main results of this discussion which I will not be repeating over here. But I would like to draw your attention to this part which I will touch upon.

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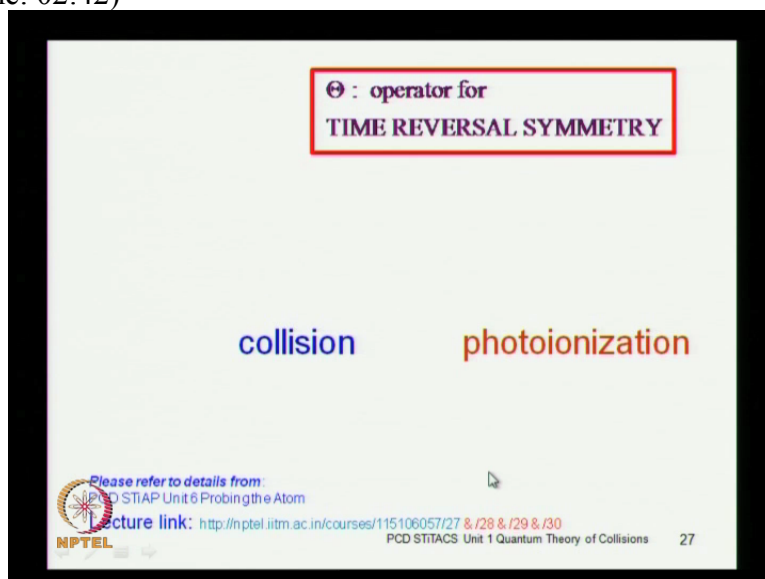


So, people who do photoionization physics and electronic scattering or anything in quantum collisions they use the same quantum theory, the same tools in quantum theory because these two processes photoionization and scattering are related to each other through the time reversal symmetry and if you recall a discussion on this diagram.

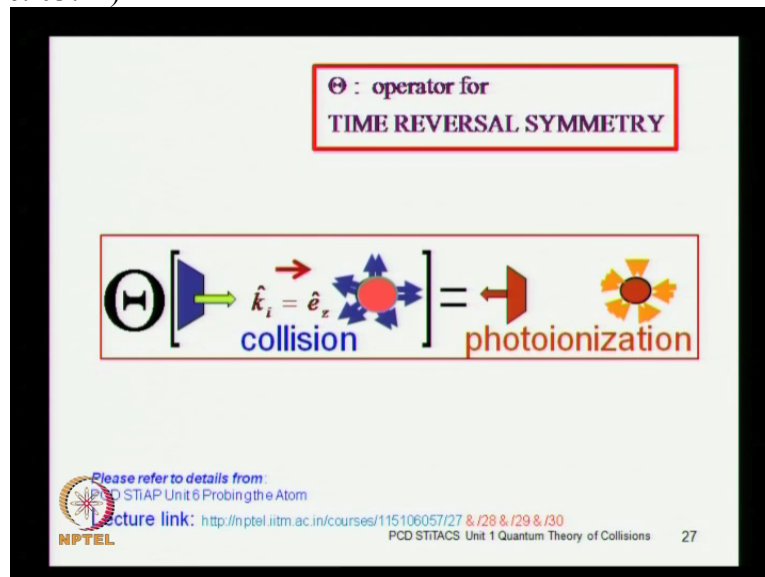
You can have a neutral atoms over here A is a neutral item when it absorbs a photon $h\nu$ you get an excited state a complex which can decay into an electron and ion but you can reach this particular fragments, electron and ion by starting out with completely different ingredients.

By starting out not with the photon and an atom but starting out by electron and ion through electron ion scattering. So, you can get the same final state but the initial states are completely different.

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And these two processes which are collision and photoionization. They are related to each other by the time reversal symmetry operator and the physics of this relationship is something that you will find in these four lectures at this link. So, I will not repeat the details over here. (Refer Slide Time: 03:11)



The results of this time reversal symmetry is that you get photoionization as a process which is time reverse of collision. So, in collision you have got an incident plane wave, so this is the incident plane wave which is moving from left to right and I consider the left to right direction as the direction of the z axis. So, the unit vector \hat{e}_z is along this, the momentum vector \hat{k}_i is along the z axis.

And this plane wave interacts with the target potential which is centered over here and you have an outgoing spherical wave as a result of this scattering. So this is what you get in a collision experiment. In a photoionization experiment you do not have an electron in the initial state at all. You just have an atom which absorbs an electron and as a result of energy conservation subject to certain selection rules angular momentum and so on.

The electron escapes into the continuum and it escapes as a free electron represented by a plane wave. So, the exit channel the escape direction is unique in photoionization and you can simulate the initial state by a spherically in going wave as we have discussed in details in these four lectures away a lecture number 27, 28, 29 and 30 at this link.

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Θ : operator for
TIME REVERSAL SYMMETRY

$\psi_{Tot}^+(\vec{r}, t) \xrightarrow{r \rightarrow \infty} e^{+i(kr - \omega t)} + \frac{e^{+i(kr - \omega t)}}{r} \left\{ \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [e^{2i\delta_l(k)} - 1] P_l(\cos \theta) \right\}$

collision $\hat{k}_i = \hat{e}_z$ **photoionization**

$\psi_{Tot}^-(\vec{r}, t) \xrightarrow{r \rightarrow \infty} e^{+i(kr + \omega t)} + \frac{e^{+i(kr + \omega t)}}{r} \left\{ \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [e^{2i\delta_l(k)} - 1] P_l(\cos \theta) \right\}$

Please refer to details from PCD STITACS Unit 6 Probing the Atom
Lecture link: [http://nptel.iitm.ac.in/courses/115106057/27 & 28 & 29 & 30](http://nptel.iitm.ac.in/courses/115106057/27%20&28%20&29%20&30)
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The net result of this is that you get a solution corresponding to outgoing wave boundary conditions and solution with reference to what are called as in going way boundary conditions. And these two are the boundary conditions which you impose on the quantum mechanical problem and they give you different solutions and the time dependent solution for scattering is what you find in this blue loop.

And that solution for photoionization is what you found in this lower loop okay so these are the two solutions. Now with reference to this analysis our focus in this course, at least in this unit is going to be on collisions in which we make use of the outgoing wave boundary conditions outgoing wave boundary conditions which are represented by this superscript plus sign over here.

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

$\vec{j}(\vec{r}) = \frac{\hbar}{2mi} [\psi^*(\vec{r}) \vec{\nabla} \psi(\vec{r}) - \psi(\vec{r}) \vec{\nabla} \psi^*(\vec{r})]$ Probability current density vector
 $= \text{Re} \left\{ \frac{\hbar}{mi} \psi^*(\vec{r}) \vec{\nabla} \psi(\vec{r}) \right\}$

$\text{incident } \vec{j}(\vec{r}) = \text{Re} \left\{ \frac{\hbar}{mi} A(k)^* e^{-ikz} \times \left[\hat{e}_x \frac{\partial}{\partial x} + \hat{e}_y \frac{\partial}{\partial y} + \hat{e}_z \frac{\partial}{\partial z} \right] \left\{ A(k) e^{ikz} \right\} \right\}$

$\text{incident } \vec{j}(\vec{r}) = |A(k)|^2 \frac{\hbar \vec{k}_i}{m} = |A(k)|^2 \vec{v}_i$ δz
 $\vec{v}_i = \frac{\delta z}{\delta t}$
 $\delta S \delta z = \delta V$

$\text{incident } \vec{j}(\vec{r}) \cdot \vec{\delta S} = \vec{j}(\vec{r}) \cdot \delta S \hat{e}_z = |A(k)|^2 v_i \delta S = |A(k)|^2 \frac{\delta z}{\delta t} \delta S = |A(k)|^2 \frac{\delta V}{\delta t}$ current through area δS

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And the solution without going way boundary condition to the quantum collision problem is that the total solution is given by the incident plane wave plus a scattered spherical outgoing

wave the $1/r$ takes care of the fact that the amplitude must diminish as $1/r$. So, that the intensity would diminish as $1/r^2$ because in a spherically outgoing wave the same flux will go through a solid angle and when it intersects a sphere okay.

The area of a sphere we know increases, increases as r^2 . So, that is taken care of by the $1/r$ factor but then there is a scattering amplitude which must have the dimensions of length okay. So, the problem is scattering theory really boils down to determining these scattering amplitudes and the phase shifts and so on.

Now what I am going to refer to is the probability current density vector which you would have met in your first course in quantum mechanics. Now this is what the probability current density vector is okay. Now we will study this current density vector in the context of the scattering solution with outgoing wave boundary conditions.

So, you have got the incident wave there is a certain amplitude which depends on the energy and the dependence on energy is manifest through the argument k because energy is $\hbar^2 k^2 / 2m$ right. So, k is a parameter which tells us what the energy is, so there is an energy-dependent normalization A_k and the current density vector corresponding to the incident wave alone.

This is the total wave function which is a superposition of the incident wave and the scattered spherical outgoing wave according to the outgoing wave boundary conditions okay. The current density vector corresponding to the incident wave alone will be given by this $\hbar / m i \Psi^* \nabla \Psi$ where in the Ψ that you are going to plug in is only the incident wave which is this e^{-ikz} okay along with the normalization A_k .

So this is the $\hbar / m i$ then you have got the complex conjugate of this part so this becomes $A^* e^{+ikz}$ okay. And then you have the gradient of the wave function, so the gradient operator in Cartesian is this which operates on the incident plane wave along with the energy dependent normalization. So, let us examine what is this incident current density vector corresponding just to the incident wave part.

We will also study the scattered part and also the interference term. So, our first focus is on the current density vector, the probability current density vector with reference to the incident wave alone. And this as you can see this wave function depends only on z , so partial derivatives with respect to x and y will vanish.

So, you have got only the e_z component and from the derivative of this with respect to z you get i_k and the numerator i will cancel this denominator i and you get $\hbar \mathbf{k}$ over m , which is really the velocity okay, momentum by the mass. So, this is your incident current density vector, what is the actual flux going through a certain cross sectional area so you have got an incident beam okay.

You have got an electron gun or you know your projectiles are being fired from a certain source you are carrying out a certain scattering experiment what a target the incident plane wave is coming in, in a certain direction okay. And then a certain amount of it is crossing some area okay per unit time. So, what is the flux which is crossing a cross section area which is Δs and you consider this Δs to be orthogonal to the direction of incidence.

So, you will represent this area with as an elemental vector area with a direction pointing in the same direction as the incident beam okay. So, this is the area and we examine what is the current through this area. So, this will be just the dot product of the current density vector with the elemental vector area Δs which you can see.

Since $\mathbf{j} \cdot \mathbf{e}_z$ is A_k square modulus of A_k squared times velocity multiplied by the area because these two are in the same direction, so both give you an $e_z \cdot e_z$ which is unity. So, now this is the picture you have this is the elemental area you have got incident flux coming from this side it crosses this one at a velocity v_i okay.

That velocity is Δz by Δt right, what is the distance covered along the positive z direction is the velocity of the beam. So, this velocity is Δz by Δt , so this is the size Δz , this is the magnitude of Δz . This is how much this cross sectional plane will advance through in time Δt .

And it will sweep a certain volume which is this as you see in this figure right. So, at this incident, when it is incident on the first surface in a direction along positive z axis at a velocity v_i , which is Δz by Δt , so in time Δt it will sweep a certain volume which is, what you see in this figure.

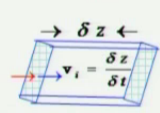
And this incident current through the area Δs you can now write as v_i written as Δz by Δt but Δz multiplied by this cross section area Δs is actually the volume. So you get Δv by Δt , where this is an infinitesimal volume under consideration. So, this is the current through area Δs okay.

(Refer Slide Time: 13:10)

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

$$\text{incident } \vec{j}(\vec{r}) = |A(k)|^2 \frac{\hbar \vec{k}_i}{m} = |A(k)|^2 \vec{v}_i$$

$A(k) = 1 \rightarrow \left[\text{incident } \psi = e^{i\vec{k}_i \cdot \vec{r}} \right]$
 Probability density $\rightarrow \psi^* \psi = 1$
 Current density: $\text{incident } \vec{j}(\vec{r}) = \frac{\hbar \vec{k}_i}{m} = \vec{v}_i$



$$\text{incident } \delta \Phi_{\text{through area } \delta S} = \text{incident } \vec{j}(\vec{r}) \cdot \overline{\delta S} = \vec{j}(\vec{r}) \cdot \delta S \hat{e}_z = v_i \delta S = \frac{\delta z}{\delta t} \delta S = \frac{\delta V}{\delta t}$$

Density of particles: 1 particle per unit volume;
 i.e. 1 particle x-ing unit area in unit time at velocity $\vec{v}_i = v_i \hat{e}_z$

incident flux per unit area: ${}^i \delta \Phi = v_i$

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Now having considered the incident current through area delta s, let us ask what this would correspond to if the normalisation, the energy dependent normalization is chosen to be one okay. This is not mandatory but it is just to keep track eventually, we will find that this normalization is not particularly important. But at this stage, let us ask what this normalization will lead us to.

So, incident wave which is A times e to the ikz will be only A being equal to 1, it will be only e to the ikz or e to the ik dot r, so that is your incident wave. So, the probability density is Psi star Psi which is unity okay. This is of course not square integrable as we know and we have discussed the normalization of continuum functions in the previous course but we will come back to that at an appropriate juncture.

Let us consider the current density which is h cross k over m, which is just the velocity itself okay, its magnitude will be the same as that of the velocity. And the flux through area delta s which is this j dot delta s this will be equal to this velocity times the cross sectional area which we know gives us the rate of change of this volume okay delta V by delta t.

Essentially what it means is that this particular choice of normalization Ak equal to 1, if this is a choice if we make this choice what this choice corresponds to is a certain density of particles. Because delta V by delta t tells us that there will be one particle per unit volume. So, that it will cross unit area in unit time at this particular velocity. So, given the initial velocity which depends on the energy of the incident beam?

Energy of the incident beam is h cross square k square by 2m, h cross k by m is the velocity and with reference to that velocity which is vi you get one particle per unit volume with this choice of normalization. On the incident flux per unit area this is the flux in area delta S. So,

if you divided by the area delta S, you get v itself. So, this is what this normalization corresponds to sorry, this is delta v by delta t okay.

So, in that entire volume how much a volume is swept in delta t okay? Now if this is unity if delta V by delta t is unity, you have one particle in unit volume corresponding to one particle crossing unit area. So, if you have got a very intense source okay, which is generating a large number of incident projectiles? Then all of these will crowd into that volume that you are talking about. And you will have more particles in the unit volume.

If you reduce the intensity this number can go down, it can go down from 100 to 10 to 1 maybe even less than 1 that you will need not just one second, not just one unit of time but maybe in two units of time you will find a particle. So, that is something that you are going to control. So, this particular choice of normalization that when delta V by delta t is equal to unity. You will get one particle crossing unit area per unit time.

So, one particle in that unit volume that is the normalization that is indicated by this energy dependent normalization $Ak = 1$. Nevertheless in our discussion we will find that the results which are of importance to our discussion they will be independent of the normalization but that is something that you will see as we proceed.
(Refer Slide Time: 17:41)

The slide contains the following mathematical derivations:

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

scattered part $\psi_{k_i}^+(\vec{r}; r \rightarrow \infty) \rightarrow A(k) \left[\frac{f(\hat{\Omega})}{r} e^{ikr} \right]$

$$\vec{j}(\vec{r}) = \text{Re} \left\{ \frac{\hbar}{mi} \psi^*(\vec{r}) \nabla \psi(\vec{r}) \right\}$$

$$\vec{j}(\vec{r}) = \text{Re} \left\{ A(k)^2 \frac{\hbar}{mi} \left[\frac{f^*(\hat{\Omega})}{r} e^{-ikr} \right] \left[\hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{e}_\phi \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \right] \left[\frac{f(\hat{\Omega})}{r} e^{ikr} \right] \right\}$$

$$\frac{1}{r} \frac{\partial}{\partial \theta} \left[\frac{f(\hat{\Omega})}{r} e^{ikr} \right] \rightarrow O\left(\frac{1}{r^2}\right)$$

$$\frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \left[\frac{f(\hat{\Omega})}{r} e^{ikr} \right] \rightarrow O\left(\frac{1}{r^2}\right)$$

$O\left(\frac{1}{r^2}\right)_{r \rightarrow \infty} \rightarrow \text{ignore w.r.t. } O\left(\frac{1}{r}\right)$

$$\vec{j}(\vec{r}) \approx \text{Re} \left\{ |A(k)|^2 \frac{\hbar}{mi} \left[\frac{f^*(\hat{\Omega})}{r} e^{-ikr} \right] \hat{e}_r (ik) \left[\frac{f(\hat{\Omega})}{r} e^{ikr} \right] \right\}$$

$$= |A(k)|^2 \frac{\hbar k}{m} \frac{f(\hat{\Omega})^2}{r^2} \hat{e}_r$$

NPTEL logo and PCDS TITACS Unit 1 Quantum Theory of Collisions 30

So, this is what you have got this is the total wave function we consider the current corresponding to the incident wave. Let us consider the scattered part now. The scattered part is the second term which is the scattering amplitude divided r times e to the ikr, which is here and this is also scaled by the same energy dependent normalization right.

So this is the scattered part in the total wave function, what is the current density corresponding to the scattered part. You have got a similar expression this is the general expression for the probability current density vector and we specialize this to the scattered part alone.

So, you have got a $\Psi^* \nabla \Psi$, so from this you will get $A^* \nabla A$ coming from here, $A \nabla A^*$ so that is the modulus A^2 . You have got this $\hbar \nabla \psi$ coming from here and then you have got the complex conjugate of this part. So, you have got $f^* e^{-ikr}$ and then you have got the gradient of the function itself which is $f e^{ikr}$.

It is scaling through the normalization constant A has already been taken into account over here okay. So this is your scattered part current density vector. If let us look at these two terms they involved they are coming from the gradient operator and they correspond to the derivative of the scattered part of the wave function with respect to the angles θ and ϕ the polar angle and the azimuthal angle.

And if you look at these two terms you will see immediately that this term is of the order of $1/r^2$. There is $1/r$ here, there is $1/r$ here and it will be of the order $1/r^2$ is the same with the derivative with respect to the azimuthal angle okay. That you have a term $1/r$ here, another $1/r$ here and it will go as $1/r^2$.

So, in the asymptotic region where you carry out your detection where your detector is located, $1/r^2$ terms will not be of any significance in comparison with the $1/r$ term. Whenever you make an approximation it is always in comparison with some other terms and there are leading terms of the order $1/r$ with reference to which in comparison with which the $1/r^2$ terms will be ignored.

So, we will ignore $1/r^2$ in the asymptotic region which we refer to as are tending to infinity with respect to terms of the order of $1/r$. So, O stands for the order okay, so these are terms of the order $1/r^2$ and these terms we ignore with respect to or in comparison with terms of the order $1/r$. And to this approximation and this is the approximation that we will apply throughout our analysis.

The scattered part of the current density vector I have used a nearly equal to sign over here just because I want to remind at the beginning that this is an approximation in which you are ignoring terms of $1/r^2$. But later on we will put equality because we will have accepted that approximation.

So, this scattered part of the current density vector will be the real part of this complex conjugate of the function which is $f^* e^{-ikr}$. These two terms are making no contribution okay, because their contributions are of the order $1/r^2$. So the only contribution you get is from the partial derivative with respect to r and when you take the partial derivative with respect to r of e^{-ikr} by r .

The only term you need to consider is the derivative of e^{-ikr} because the derivative of $1/r$ will again be of all over $1/r^2$ okay. So, that term will be thrown and the only term that is under consideration is $ik e^{-ikr}$ which is coming from the derivative of e^{-ikr} with respect to r . So, this is $ik e^{-ikr}$, the other term which is of the order $1/r^2$ we have ignored once again.

So this is the scattered part of the current density vector. Now you multiply e^{-ikr} with e^{-ikr} to the $-ikr$, so these two terms cancel then there is an i here in the numerator and an i here in the denominator, so those two cancel, so you are left with the squared of the modulus of this amplitude A .

Then you have got f^* and f which will give you the square of the modulus of f right f is the complex scattering amplitude and you get its modular square. And then what as you get you get $h \times k$ there is a k here, there is a m here. So, you get $h \times k$ over m right, which is the velocity. And then there is a $1/r$ here and $1/r$ here, so you get $1/r^2$ okay.

So, that is what you have got you get the modulus of a square $h \times k$ over m squared of the modulus of the scattering amplitude $1/r^2$ along the direction, the radial direction, the unit vector e_r which is along the radial direction, it is a vector quantity this is already current density vector, it has the direction of the unit outgoing radial vector right.

So, this is the scattered part $1/r^2$ you ignore when it comes as an additive term with $1/r$. If there are two terms one of which is $1/r$, the other is $1/r^2$ and they are added to each other. Then you throw the $1/r^2$ with reference to $1/r$, if $1/r^2$ is that is there to it. You cannot throw it okay, so while making approximations you always have to be careful.

That when you say that your approximation is correct up to a certain order then it means that you are retaining leading terms to that order. But leading what so there has to be a certain series a number of terms. So, this amount of water in this bottle this can be very large compared to the amount of water in this lid right. But this is nothing if you talk about the amount of water in a river okay. Rivers go dry in Chennai that is a different story okay.

So let us not worry about that okay. So, $1/r^2$ is ignored when you are comparing it with another term which is $1/r$. And in our earlier part where we did ignore it is only because it came together with $1/r$ as an additive term. Here this is the net scattered current density vector okay.

(Refer Slide Time: 25:24)

The slide contains the following text and equations:

- incident flux per unit area:** $\delta\Phi = |A(k)|^2 v_i$
- scattered part:** $\vec{j}(\vec{r}) = |A(k)|^2 \frac{\hbar k}{m} \frac{|f(\hat{\Omega})|^2}{r^2} \hat{e}_r$
- Scattered flux in the radial outward direction through elemental area $\delta S = r^2 \delta\Omega$**
- scattered part:** $\delta\Phi = \vec{j}(\vec{r}) \cdot \delta S \hat{e}_r \approx |A(k)|^2 \frac{\hbar k}{m} \frac{|f(\hat{\Omega})|^2}{r^2} \hat{e}_r \cdot \delta S \hat{e}_r$
- scattering amplitude:** $[f(\hat{\Omega})] \rightarrow L$
- scattering amplitude:** $|f(\hat{\Omega})|^2 \rightarrow L^2$

At the bottom left is the NPTEL logo. At the bottom center is the text "PCD STITACS Unit 1 Quantum Theory of Collisions". At the bottom right is the page number "31".

So, the incident flux per unit area we determined earlier which was modulus A square times v_i you remember that this result we got earlier. The scattered part we have now got which is mod A square \hbar cross square k by m and mod f square by r square times the unit vector right. This is the scattered part of the current density. So, the scattered flux through this elemental area.

So, this is the scattered direction, this elemental areas subtend a solid angle $\delta\Omega$ at the center. We have used these figures earlier also in our previous class. So, this $\delta\Omega$ subtends these surface δS , subtends a solid angle $\delta\Omega$ at the center. So, this δS is r square $\delta\Omega$.

So, this being the current, the net flux through this area will be \vec{j} dot this elemental area vector which is δS times the outward unit normal to this \vec{e}_r . What is this it is \vec{e}_r dot \vec{e}_r will give you 1 and then you have the rest of the terms coming from this A square \hbar cross square k over m , which is here f squared over r square is here and \vec{e}_r dot \vec{e}_r is here, this elemental area δS is here right.

So, this is your scattered part of the flux. Now you can ask the, you can make a comparison between the scattered flux and the incident flux but you certainly know that this quantity has

got the dimensions of length. So, this term goes as l square modulus of f square has got the dimensions of l square.
 (Refer Slide Time: 27:33)

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

incident flux per unit area: $i\mathcal{D} = A(k)^2 v_i$

Scattered flux in the radial outward direction

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

$$\frac{s\mathcal{D}}{i\mathcal{D}} = |f(\hat{\Omega})|^2 \delta\Omega \quad |f(\hat{\Omega})|^2 : L^2 \quad \frac{d\sigma}{d\Omega} = \lim_{\delta\Omega \rightarrow 0} \frac{\delta\sigma}{\delta\Omega} = |f(\hat{\Omega})|^2$$

scattering x-sec per unit solid angle differential x-sec

This definition is independent of the normalization

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And you have got the incident flux you have got the scattered flux okay. In the scattered flux you have got r square in the denominator and r square in the numerator, so they cancel each other. And now you ask; what is the ratio of the scattered flux to the incident flux so, how much of scattered flux do you get per unit incident flux that is the question you are asking. It is going to be a measure of the probability of scattering right.

How much of scattering is taking place so what the target is doing is it takes a certain part of the incident flux interacts with it and scatters it and that part which is scattered is removed from the incident flux okay. Because no new particles are created or destroyed so there is a conservation of the total amount of matter that is there.

So, whatever is coming in a certain part of it is being picked and scattered into various regions just the way optical scattering takes place okay. That an object which obstructs an incident beam of light will take some of the incident intensity and scatters it in different directions so behind it there will be a shadow.

And there will be scattering of the some part of the incident beam although some of the incident beam can actually go through depending on the transmission probability. So, what is the value of this ratio you got both the terms you have got the incident flux is this, the scatter flux is this. So, you just have to divide this right hand side of this by the right hand side of this. So, modulus A square is common in both when you take the ratio that will go off.

The magnitude of the velocity is common in both. There is a velocity here there is h cross k over m over here. So these terms will also cancel each other when you take the ratio right. So, what is the ratio giving you the ratio will give you only this term, square of the modulus on the solid angle $d\Omega$?

So, if you now take this ratio per solid angle per unit solid angle divided it by the solid angle. You will get the scattering probability per unit solid angle. So that is what is called as differential scattering cross section okay. It is $d\sigma$ by $d\Omega$ in the limit $d\Omega$ going to 0; we already recognized that the scattering cross section it will have the dimensions of l^2 which is coming out right.

We discuss the dimension in our previous class of the scattering cross section right, which has got the dimensions of l^2 . These dimensions are correctly preserved as we expect that to happen that is a necessary feature of this analysis. And the term that is coming in is the square of the modulus of the scattering amplitude, the complex scattering amplitude which has got the dimension of length.

So, this is the differential scattering cross section and the normalization energy dependent normalization does not appear anywhere in this description. So, it really does not matter which is what I had hinted earlier. But now you can see clearly that this particular result that $d\sigma$ by $d\Omega$ is given by the square of the modulus of the scattering amplitude is completely independent of the energy dependent normalization.

So, this is scattering cross section per unit solid angle you have divided it by the solid angle $d\Omega$. So, it is a cross cutting cross section per unit solid angle which is why this called is the differential cross section.

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

Probability current density vector

$$\vec{j}(\vec{r}) = \frac{\hbar}{2mi} [\psi^*(\vec{r}) \nabla \psi(\vec{r}) - \psi(\vec{r}) \nabla \psi^*(\vec{r})]$$

$$= \text{Re} \left\{ \frac{\hbar}{mi} \psi^*(\vec{r}) \nabla \psi(\vec{r}) \right\} \quad \psi: \text{total wavefunction}$$

Radial component of the probability current density vector

$$\vec{j}(\vec{r}) \cdot \hat{e}_r = \text{Re} \left\{ \frac{\hbar}{mi} A(k)^* \left[e^{-i\vec{k}_i \cdot \vec{r}} + \frac{f^*(\hat{\Omega})}{r} e^{-ikr} \right] \times \left[\hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{e}_\phi \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \right] \left\{ A(k) \left[e^{i\vec{k}_i \cdot \vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr} \right] \right\} \right\} \cdot \hat{e}_r$$

$$\vec{j}(\vec{r}) \cdot \hat{e}_r = \text{Re} \left\{ \frac{\hbar}{mi} |A(k)|^2 \left(e^{-i\vec{k}_i \cdot \vec{r}} + \frac{f^*(\hat{\Omega}) e^{-ikr}}{r} \right) \frac{\partial}{\partial r} \left(e^{i\vec{k}_i \cdot \vec{r}} + \frac{f(\hat{\Omega}) e^{ikr}}{r} \right) \right\}$$

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And we now consider the probability current density vector corresponding to the full wave function what we did so far was to consider just the incident part first. Then we considered just the scattered part. We now consider the probability current density vector corresponding to the complete wave function.

So, what is going to go in this expression for the probability current density vector, the Psi star will be a complex conjugate of both of these terms and the gradient will be taken of this entire wave function inclusive of both the terms. So let us do that but we will focus our attention on the radial component of this current density vector.

So, take the current density vector take its radial component which is j dot er okay, j know is given by this expression in which Psi star is the complex conjugate of this. So, you begin with this h cross over mi coming from here, then you have the complex conjugate of this wave function so you got A star and e to the -ik dot r f star over r e to the -ikr this is the complex conjugate of this wave function.

Then you got the gradient operator and then you got the wave function itself which is the incident part plus the scattered part normalized according to the energy dependent normalization okay. So, this is the radial component of the current density vector. So, let us evaluate this term now, how do you do that, mind you that after taking all these derivatives you have to take a dot product with this radial unit vector.

So, all terms in which you have got er dot e theta or e phi will vanish okay. Because they are orthogonal unit vectors er, e theta, e phi constitutes a right handed orthogonal system of practice basis vectors. So, the only term that you will read to consider is the one in which you

have got the unit vector \hat{e}_r which dotted with this \hat{e}_r will give you 1 okay. The other terms will not contribute.

So, you have just the partial derivative with respect to r coming from this operator $\hat{e}_r \cdot \nabla$ by $\nabla \cdot \hat{e}_r$. And then you have got this wave function the incident part plus the scattered part this amplitude together with the complex conjugate over here gives you the modular square over here that is taken care of. So, this is your expression for the radial component of the current density vector corresponding to the total wave function okay.
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$$\vec{j}(\vec{r}) \cdot \hat{e}_r = \text{Re} \left\{ \frac{\hbar}{mi} |A(k)|^2 \left(e^{-i\vec{k}_i \cdot \vec{r}} + \frac{f^*(\hat{\Omega}) e^{-ikr}}{r} \right) \frac{\partial}{\partial r} \left(e^{i\vec{k}_i \cdot \vec{r}} + \frac{f(\hat{\Omega}) e^{ikr}}{r} \right) \right\}$$

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

$O\left(\frac{1}{r^2}\right)_{r \rightarrow \infty} \rightarrow \text{ignored w.r.t. } O\left(\frac{1}{r}\right)$
 Radial component of the probability current density vector

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

$$= \text{Re} \left\{ \frac{\hbar}{mi} |A(k)|^2 \left[e^{-i\vec{k}_i \cdot \vec{r}} (ik) \frac{f(\hat{\Omega}) e^{ikr}}{r} + \frac{f^*(\hat{\Omega}) e^{-ikr}}{r} (ik \cos \theta) e^{i\vec{k}_i \cdot \vec{r}} \right] \right\}$$

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Now this total wave function you can break this current density, this current density is made up of three parts, one is a pure incident part which we have evaluated separately. There is one corresponding to the outgoing scattered part which also we have evaluated separately. And then there is also an interference term but while doing this analysis we are throwing the $1/r^2$ terms okay.

With reference to comparison with $1/r$, so if you now consider the interference term because the pure incident term and the pure scattered outgoing term. We have already considered. Let us now consider the interference term but we will focus on the radial component of the interference term. So, this is the component of the current density vector corresponding to the interference term.

And the component along the radial outward direction \hat{e}_r , so the interference will come from the incident plane wave and an outgoing scattered wave over here. So, this is $e^{-i\vec{k}_i \cdot \vec{r}}$ $\nabla \cdot \hat{e}_r$ of this term is what will contribute to the interference term right. Then this term pre multiplying the partial derivative of the incident wave will also contribute to the interference term.

So, these are the two terms underscored by the blue and the red which contribute to the interference term right. So, let us get them, so you got \hbar cross over m square of the modulus of A . Then you have got A to the $-ik \cdot r$, which is the incident wave and the derivative with respect to r of the scattered outgoing wave that is coming from the first interference term.

The second interference term is this factor the scattered outgoing wave rather the complex conjugate of the scattered outgoing wave pre multiplying the partial derivative with respect to r of the incident wave e to the $ik \cdot r$, so these are the two terms. So, let us get these derivatives, when taking these derivatives again you will get an ik coming from the derivative of e to the ikr .

You will also get a term in 1 over r square coming from the derivative of 1 over r which you will ignore okay. So, when you work within that approximation you can consistently ignore 1 over r square in comparison with 1 over r . Your interference term then have this term ik is coming from the derivative of e to the ikr when you take the derivative with respect to r . So, you get ik , then you get $f e$ to the ikr by r .

And from the second term you get $f^* e$ to the $-ikr$ by r which is coming from here and then you need a derivative with respect to r of e to the $ikr \cos \theta$ okay, θ being the angle between incident wave and the radial direction. So that is what will give you $ik \cos \theta$ when you, because the derivative is with respect to 1 okay, what we have done is to ignore 1 over r square.

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Radial component of the probability current density vector

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

$$= \text{Re} \left\{ \frac{\hbar}{mi} |A(k)|^2 \left[e^{-i\vec{k}_i \cdot \vec{r}} (ik) \frac{f(\hat{\Omega}) e^{ikr}}{r} + \frac{f^*(\hat{\Omega}) e^{-ikr}}{r} (ik \cos \theta) e^{i\vec{k}_i \cdot \vec{r}} \right] \right\}$$

$O\left(\frac{1}{r^2}\right) \xrightarrow{r \rightarrow \infty}$ ignored w.r.t. $O\left(\frac{1}{r}\right)$

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

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So, these are the two terms that you get for the radial component of the probability current density vector coming from the interference term. Now there is an ik here which we got from here, there is also an ik here. So you can take this ik factor it out as a common factor then you

will be able to cancel this i in the numerator with this i in the denominator you will also get h cross k over m as the velocity.

And then you have rather similar looking terms inside this rectangular bracket. You got f over out here, here you have got f start over r , you have got an additional cosine theta over here. You got e to the $+ikr(1-\cos\theta)$ but we have here e to the $-ikr(1-\cos\theta)$ okay. So, keep track of the signs very carefully. So, you cancel this i , this i cancel this i in the denominator. (Refer Slide Time: 40:38)

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

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


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

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

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


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

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



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



And after the cancellation of that i you get this h cross k over m . And these are the two terms now at this point you need to recognize a fact that your incident beam will not be very strictly mono energetic, the energy will have a little bit of spread okay. You never have a strict mono energetic beam. So, corresponding to the spread in energy the value of the momentum which is k , E is h cross square k square by $2m$.

So, k is directly determined by the energy and when the energy is not strictly mono energetic, k will have a certain spread. So the values of k will change from k to $k + \Delta k$ and whatever expressions you have over here for completeness, you will then have to carry out an integration over k .

Because there will be contributions from all values of k between k and k plus Δk , some range whatever it is, its value is not very significant, it will be a narrow range nevertheless it will not be a sharp energy. So, let us see the consequences of this fact that it is always present in any experiment. Because there is no experiment in which you can get a strict mono energetic beam.

To get strict mono energetic, you know even in spectroscopy, you get exactly one frequency corresponding to a transition from an upper state to a lower state only if these energy levels are infinitely sharp, which they never are, let alone broadening due to thermal effects and other causes because of collisions and so on okay.

All of this is incident particles they are also colliding with each other right. So there will be some momentum transfer amongst themselves. There will be temperature dependent terms okay. But in addition to that, yeah there is the energy time uncertainty sorry (Question time: 43:08) scattering phase shift that will have effect yeah; it will be it will get effect within that narrow range.

So it is they were strictly mono energetic and there is a minimum, no matter even if you do this experiment at zero temperature, half the incident beam so weak that there is only one particle passing in like one day or something you can reduce the intensity to that extent. So, that it has no interaction of possibility of interacting with anything else before it meets the target.

So, you can minimize all that but you can never get rid of the uncertainty the natural uncertainty ΔE okay. So there will always be a little bit of spread that is the spread that I am referring to but not only to that natural uncertainty spread. In a real experiment that is spread because of additional factors like thermal effects collision amongst each other and so on right.

All of that together gives you a net overall spread from k to $k + \Delta k$. Now when you have this spread, look at these two terms this is where k appears, this is $e^{i(kr - \omega t)}$. Here you have got $e^{i(kr - \omega t)}$. These are the terms where you are having k and this k is not unique anymore. These terms will have to be integrated from k to $k + \Delta k$ because there will be corresponding contribution from every value of k in that range.

So, you need integration from k to $k + \Delta k$ of these two terms $e^{i(kr - \omega t)}$ either with a plus sign or with a minus sign these are the two terms which I am considering together in this integral. So there is one term with the plus sign and the other time with the minus sign.

So, there are two integrals under consideration and they correspond respectively to the two terms which are k dependent or this is a very simple integral it is integral of an exponential function. So, it is exponential function divided by the rest of the terms, so it is $\frac{e^{i(kr - \omega t)}}{k}$ plus or minus right.

And you have to take the difference of this expression. You have to subtract the value at the lower limit from the value at the upper limit. The value at the upper limit you get by replacing this dummy index k prime by $k + \Delta k$. And the lower limit k prime will take the value k , so you take the difference.

This is the value at the upper limit, so k prime becomes $k + \Delta k$ at the lower limit k prime becomes k this is the difference the denominator is common this is what you get right. Now what you see in this expression numerator has got these exponential functions they are sine theta, cosine theta kind of terms right $e^{i\theta}$ is cosine theta + or $-i$ sine theta.

And cosine theta and sine theta they are restricted to the range -1 to $+1$ they are oscillatory okay. But their values are small their values remain of modulus 1 order. The denominator has got r , the numerator has got oscillatory terms of the order of 1 the denominator is r which is going to infinity okay. So, you have got one over infinity.

So, you can throw this except when cosine theta is $\neq 1$ because what you have in the denominator is not just r but also $1 - \cos \theta$ right. So, you can throw these terms except when cosine theta $\neq 1$ and when is cosine theta $= 1$, when theta is 0 theta must be 0, so theta is 0 in the direction which you call as a forward direction that is the direction of incidence itself right.

So, in the direction of forward scattering which is theta nearly equal to 0 this is the only place to with reference to which the interference terms are of any significance okay, sorry (Question time: 28:28) that side but that can be that can do to some other limit know, you have got oscillatory terms okay. But no matter what the value of theta is, no matter what the value of theta is.

The denominator r always has a value which is larger than the previous value because r is tending to infinity. So, there is end to it, possibility that the numerator go to zero, there is a possibility that the numerator goes to zero or one of the terms in the numerator goes to zero. The numerator consists of cosine term and the sine term both do not go to 0 at the same angle right.

So the only term which is of importance for the consideration of the interference term is the term corresponding to a very small angle? When theta is very nearly equal to 0 which is the direction of forward scattering okay, so any question over here, the main conclusion today is that we consider the interference term and the interference term you can consider for any angle at the end of this discussion we would have considered all angles in space.

In spherical polar coordinate system theta goes from 0 to pi, Phi goes from 0 to 2pi right. So, you must integrate over all azimuthal angles Phi going from 0 to 2pi. All polar angles theta going from 0 to pi, but the integration over the polar angle need not be restricted to the entire range 0 to pi because only the forward direction is of significance.

So, we need to consider scattering in a small cone in the forward direction. So, far as the discussion on the interference term is concerned okay. This part is focused on the interference term; this is the current density corresponding to the interference part of the wave function. We considered you remember how we constructed this, so we had the incident part and the derivative of the scattered part.

Then we also had the scattered part and the derivative of the incident part. So these are the two contributions to the interference term but the interference term is of significance only with reference to the forward scattering amplitude. So this is the major conclusion and we will pick up the discussion at this point in the next class any other question yes.

(Question time: 51:23) When we integrate the forward scattering once dimension of the overall get affected one over r, no because you always do it in a consistent manner, you are adding up these terms but then you will also averaged over all the energies okay. So you add the contributions over all the different energies and then averaged over them.

So, when you do the averaging you will have an energy denominator term which will take care of the dimensions okay. Your point is quite appropriate, so it is in anticipation of the fact that a incident beam will not have a strict single energy. But it will have a certain spread. In anticipation of this result we recognize the fact that the interferences term is of importance only for forward scattering.

This plays an important role in the derivation of the optical theorem which we are about to get but we need some more time, so we will do it in tomorrow's class. Any other question (Question time: 52:47) actually I mean the conservation will be holding there, yeah for the energy for the flux conservation the complete current density vector is involved okay.

I am going to use the equation of continuity in the next class okay which is the divergence of the current density vector will be the negative partial derivative of the probability density itself right. So that is the energy you know equation of continuity which is applicable in fluid dynamics or in any current discussion.

So whenever you have this consideration the current density is made up of this $\Psi^* \nabla \Psi$, whereas Ψ is the total wave function. So, what goes into the conservation of flux is the total wave function which is why it is mandatory that you consider the interference term. So you consider the incident part, you consider the scattered part but you must also consider the interference term.

Because $\nabla \cdot \mathbf{j} = -\partial \rho / \partial t$ provided \mathbf{j} is made up of $\Psi^* \nabla \Psi$, other than that $\hbar \nabla \times \mathbf{m}$, wherein that is the total wave function which includes the incident part and the scattered okay. Okay so let us conclude today's class over here and we begin from here in the next class.