

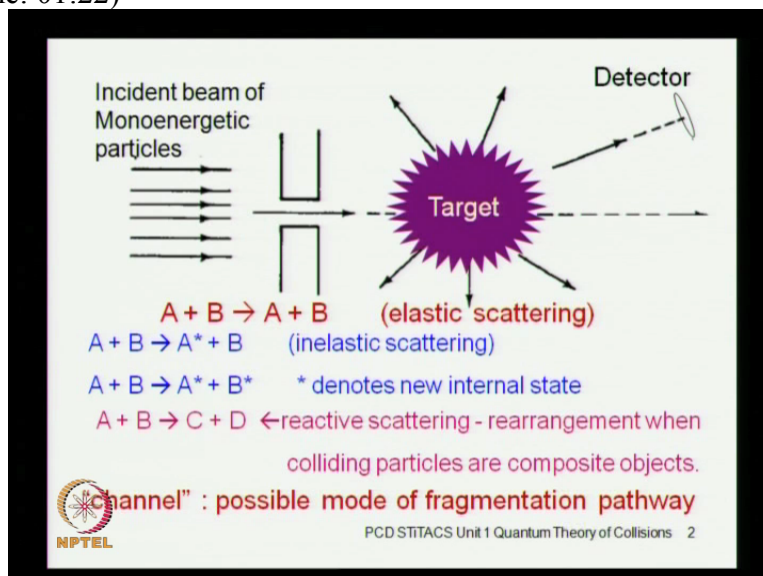
Select/Special Topics in ‘Theory of Atomic Collisions and Spectroscopy’
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Lecture 02
Quantum Theory of collisions

So, welcome to the course theory of atomic collisions and spectroscopy and again the subject is vast. So, we will only be touching select topics. The first unit will be on Quantum Theory of Collisions and we will begin with a little bit of review of collision dynamics much of it you would have learnt in your earlier courses in quantum mechanics or atomic physics. So, this will be a very quick review of some of those things.

A reminder for you to recapitulate on some of the essential results and this unit will be based on the first four chapters from the book Quantum Theory of Collisions by Charles J Joachain which is really a very nice book. And I will refer to the first four chapters of this book for unit 1 and then of course as the course progresses for other units I will give you know different source material.

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Now collisions and spectroscopy we will learn that they are you know aspects of the same phenomenon as such it depends on how you look at it. But before I get into those details let me consider a collision process. So, you have got a certain target, you want to study the target properties so you need a probe and you bombard this target by a certain projectile okay. So, you have a mono energetic beam incident beam of projectiles.

So, you have got the collimator and all these arrangements right. So, this is just a schematic diagram and then the scattered particles you detect in a detector and then from your

observations you try to seek information about the target that is the object of this experiment. And quantum theory would simulate this process.

And provide us with a rigorous mathematical description of this process which will help us analyze the results of the scattering experiment. Now there can be different kinds of you know results from this experiment, one is that if the projectile is what you call as A and the target as B. Then the two together will remain the same as they were before the experiment okay.

So, this will be elastic scattering there will be some kinetic energy transfer from one to the other, momentum transfer from one to the other. But this internal state of A and B will not change in this. So, this is the elastic scattering. You may also have some conversion from the kinetic energy to internal energy. And you may get as a result of this collision one of the atoms in an excited state or both the atoms in the excited state okay.

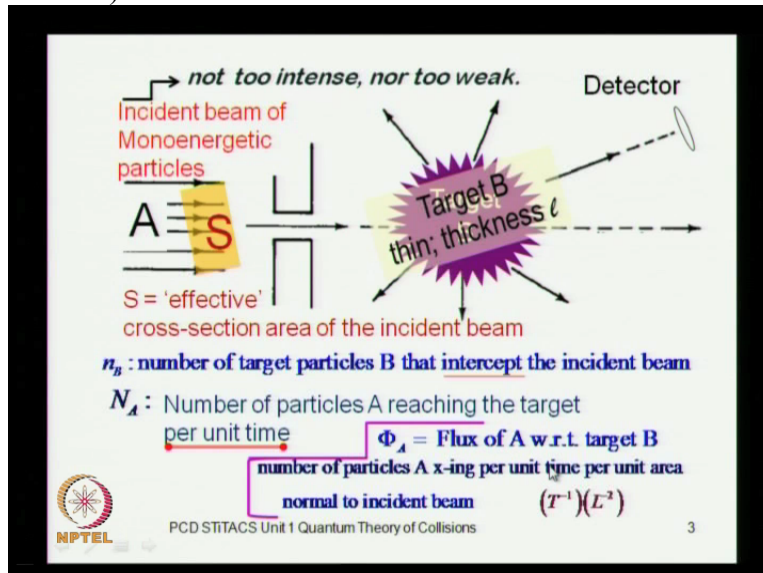
So, this could also happen and this would be inelastic scattering okay. Then you can also have reactive scattering. If A and B are composite objects. If A is not an elementary particle then it could fragment as a result of the scattering and you may get a completely new species. In fact you may get more than two resulting species.

So C and D are just symbolic, but the suggestion here is that the result of this scattering gives you species which are different from what you started out with. So, you can have reactive scattering which involves rearrangement when the colliding particles the target and the projectiles if they are composite particles they are not elementary particles.

If they are elementary particles of course they have nothing to fragment into. But if they are composite particles then they could you know rearrange and you have reactive scattering. Now there are these various possibilities in which this system can decay after the collision takes place. So, when the collision takes place you get a complex and that complex is the sum total of the two reactive species.

And how with decays does it decay according to an elastic channel or in inelastic channel or reactive scattering. So, there can be number of decay modes and each of these is a channel okay. Reactive scattering again can be in many different channels for example A plus B will give you C plus D, but it can also give you X plus Y where X plus Y are different from C and D okay.

So, there can be a number of decay channels likewise the excited states need not be unique there can be a number of different excited states. So the relationships that we have written on the screen are only suggestive they are generic and they tell us that there can be a large number of fragmentation pathways as a result of a collision.
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So, now let us consider this process in further detail first of all I would like to specify that the incident beam we shall consider to be not too intense and not too weak either okay. If it is too intense for example you have got a mono energetic beam of electrons. Then there are so many electrons over there because it is an intense beam okay.

That they will repel each other and move away right and collimation and everything will become very difficult. So, you do not want to beam which is extremely intense you do not want it to be too weak because if it is too weak you have so many so few events to observe that you cannot get adequate information. So, the incident beam will not be too intense nor will it be too weak.

Let us consider that a certain part of the incident beam is stopped by the target okay. So, the target is going to meet the incident beam right. And there will be a certain effective area of the target material which will block the trajectory of the incident beam. Now this is not necessarily the physical area nor is it necessarily made up of those target atoms which belong to the front most layer in the target.

Because some of the projectiles could penetrate and get stopped by the second layer or the third layer or the fourth layer okay but then everything put together a certain number of target particles will intercept the incident beam. Most of these may be from the first layer some of them could be from the second or third okay.

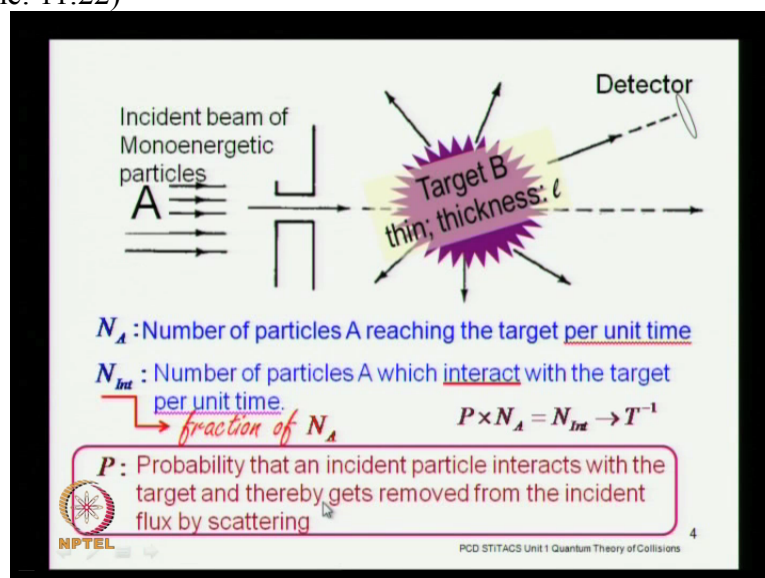
But all in all let us consider that there are there is a certain number of target particles n_B which intercept the incident beam again this interception is not just a physical interception because if these are charged particles they will have interaction at a distance and if they interact then it means that they have been intercepted by the target okay. So, it is not necessarily a physical stoppage of the incident particle but it refers to an interaction.

And a certain number of the target particles let me call this number is n_B and this number of target particles let us say it stops the incident beam and they would generate a certain effective area which is the effective cross section of the incident beam because that is what is stopped. The actual physical cross section of the incident beam need not be this okay.

So, S in our description is the effective cross section area of the incident beam okay. Now the target typically would be a thin target whose thickness let us say is this little l and I really do not know why one calls this is thickness of a thin target. I believe there is no such word as thinness. So, this is the thickness of a thin target okay and let the number of particles of the incident beam A which reach the target per unit time be given by N_A okay.

So, this is the number of particles reaching per unit time. So, N_A is a number it has got dimensions of inverse time because it is the number of particles per unit time. The flux of the incident particles the flux of A is the number of particles A crossing this x slash x dash ing is crossing okay, number of particles A crossing per unit area per unit time.

So, it will have the dimensions of inverse T and inverse L square okay. So, this is the flux of A with respect to target B which I call as Φ_A
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So, this is what we have got N_A the number of particles reaching the target per unit time and out of these N_A numbers of particles a certain fraction of these any particles will actually interact okay. They will be intercepted by the target particles all of them will not okay. Some of them will just pass through as if there was no target.

So, some of them which get stopped by the target stopped again not in the physical sense but in the sense of an interaction okay. So, a certain fraction, so N_{int} interaction is the number of particles A which interact with the target again per unit time. So N_{int} again has got the dimensions of 1 over time it is a certain fraction of N_A . So, it is less than or equal to N_A okay.

And what fraction it is will depend on the probability of interaction right because if it does not interact it is going to pass through. What is the probability of interaction will determine what is the fraction of any which will interact. So, if P is the probability of this interaction that the incident particle interacts with the target.

Then P times N_A will give you N_{int} interaction right. So, this is again a number with dimensions of inverse time okay good. Now this P is typically less than 1 often it is much less than 1 for thin targets but those are matters of quantitative details. But we certainly know that being a probability it is a number between 0 and 1.

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$N_{int} = P \times N_A \rightarrow T^{-1}$

$(T^{-1})(L^2)$
 incident flux, $\Phi_A = \frac{N_A}{S}$

n_B : number of target particles B that intercept the incident beam

How is N_{int} related to the target particles B?

$N_{int} \propto \Phi_A n_B$

What should be the dimensions of the proportionality?

$N_{int} = \sigma_{tot} \times \Phi_A n_B \rightarrow (L^2)$

$\sigma_{tot} = \frac{P \times N_A}{\Phi_A n_B}$

Scattering cross section "tendency" of particles A & B to interact
 effective target area that interacts with the incident beam and scatters it

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So, now let us ask this question that this number of interacting particles per unit time is given in terms of the number of particles of type A okay, P times N_A is N_{int} interaction right. The question is how is this number related to target particles P , N_{int} equal to P times N_A is how this interacting number of particles is related to particles A.

How is it related to particles B to the target B? Now sure enough we know that this number must be proportional to n_B because that is the number of particles which is stopping it. So, it will have to be proportional to that right. It will also have to be proportional to the flux of the incident beam right because the flux is the number of incident particles per unit area per unit time.

So, higher the flux higher do you expect the number of particles which are engaged in this interaction okay. So, N interaction will be proportional this is the symbol for proportionality it will be proportional to n_B . It will also be proportional to the flux of the incident particle and therefore any interaction will be proportional to the product Φ_A times n_B okay.

Which means that you will be able to write an equation N interaction is equal to a certain constant times Φ_A times n_B right because it is a linear proportionality, what will be the dimensions of this proportionality there will be a constant of proportionality, what will be its dimension it will have the dimensions of area right.

So that is precisely correct and the dimension of the proportionality will be an area which is called as the scattering cross section okay. It will have to be an area because n_B is just a number Φ_A has the dimensions of 1 over time and multiplied 1 over area. So, the constant of proportionality has got the dimensions of area l^2 .

This is what is called as the scattering cross section and since these two left-hand sides give you N interaction the right-hand side P into NA must be equal to σ times Φ_A into n_B . So, equating the right hand sides you get $\sigma = P$ into NA divided Φ_A times n_B and that gives you a physical interpretation of the, what the scattering cross section is okay.

So, essentially what is it telling us it is giving us a measure of the tendency of the particles A and B to interact, so it is in some sense proportional to the probability of interaction right. It is the effective area of the target which intercepts the incident beam of projectiles and scatters it okay. So, this is what the scattering cross section is.

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cross-section =

$$= \frac{\text{number of events per unit time per unit scatterer}}{\text{flux of the incident particles w.r.t. the target}}$$

$$\uparrow \sigma_{tot} = \frac{P \times N_A}{\Phi_A n_B} \uparrow$$

Scattering cross section
direction of incident beam

effective target area that interacts with the incident beam and scatters it

“tendency” of particles A & B to interact

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Now if you look at this relationship probability into N_A divided Φ_A times n_B then it tells us that the numerator is just the number of events per unit time but then there is n_B in the denominator so it is the number of events per unit time per unit scatterer right because you have divided it by n_B per unit incident flux okay.

So, that gives the physical interpretation of what the scattering cross section is. It is the number of events per unit time per unit scatterer per unit incident flux okay. So, this is the scattering cross section in quantum collision theory that we shall be talking about. (Refer Slide Time: 17:49)

effective target area that interacts with the incident beam and scatters it

Scattering cross section

scattering center

$d\sigma$

$d\Omega$

$d\theta$

1 barn = 10^{-24} cm^2 ;

1 Mega-barn = $1 \text{ Mb} = 10^{-18} \text{ cm}^2$

$$\sigma_{tot} = \frac{P \times N_A}{\Phi_A n_B}$$

cross-section =

$$\frac{\text{number of events per unit time per unit scatterer}}{\text{flux of the incident particles w.r.t. the target}}$$

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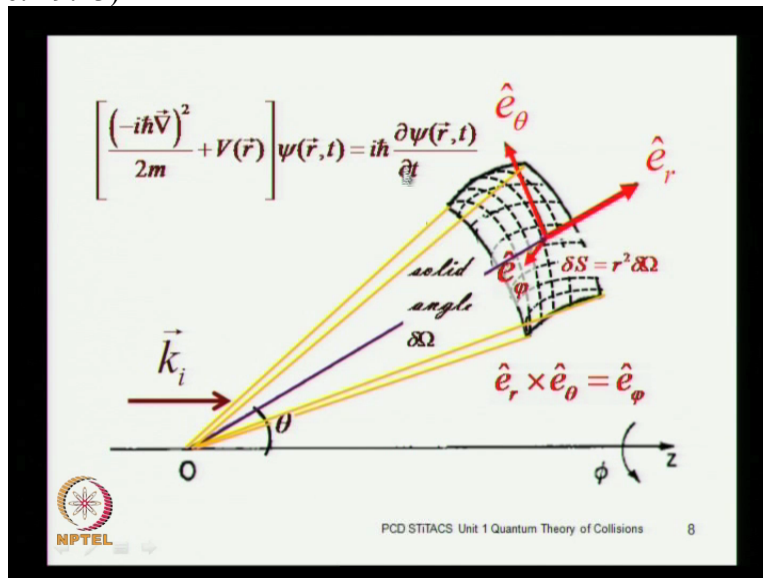
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And notice that the interaction is not just a physical stoppage but it is interaction at a distance through some electromagnetic interaction for example there will also be quantum mechanical effects because there is the exchange interaction right. So, there are all kinds of you know phenomenology not just the electromagnetic interaction.

A nuclear sketching of course there would also be nuclear you know interactions which go into the interaction Hamiltonian. So, this is an area, this is an effective area and this area is measured in units of you know some area unit is what is used the common unit to use is a barn which is 10 to the -24 square centimetre.

And very often one uses a megaborn mega is 10 to the power 6, so 10 to the power 6 of 10 to the -24 will give you 10 to the -18 square centimetre. So, this is the common unit in which the scattering cross section is reported okay. So, now let us start looking at this event in some detail so you have got an incident beam of mono energetic projectiles.

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Let us say that the momentum vector is k_i in units of \hbar , it is \hbar times k_i is the incident momentum and then it gets this particle get scattered in a certain direction and let us say that this is the radial outward direction with this center of symmetry and with reference to this incident direction as a polar axis. So, this is what we call as the z axis and angles measured with respect to z axis will be the polar angles.

So, theta would be increasing as you go away from the z axis. So, that is the polar axis and the unit vector which is orthogonal to the radial unit vector e_r which is in the direction of increasing theta is the unit vector e_θ . And the cross product of these two will give you the e_ϕ of the spherical polar coordinate system right. So if you have a little elemental area so these are tiny elemental areas that we are considering.

And this tiny elemental areas obtains a solid angle $\delta\Omega$ at the center of scattering and you have this e_ϕ which is the cross product of e_r and e_θ which gives you the azimuthal unit vector e_ϕ . So this is the geometry and the coordinate system that we shall be using. This elemental area is δS it sizes $r^2 \delta\Omega$ right.

And we want to solve the Schrodinger equation for this. That the state of the system is described by a state function Psi this is the Debralee Schrodinger wave function or you can have it written in the Dirac notation if you like. And how does the state evolve with time is the question that we are trying to answer.

So, how it evolves with time is given by its rate which is del Psi by del t and del Psi by del t is given by this Schrodinger equation. So our interest is in solving this differential equation for the scattering problem.

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The slide contains the following content:

- At the top, a diagram shows an incident wave from the left hitting a target (red circle) and scattering in various directions. A blue arrow indicates the incident wave direction, and a red arrow indicates the scattered wave direction. The wave vector is labeled $\hat{k} = \hat{e}_z$.
- The asymptotic form of the wave function is given as:

$$\psi_{\vec{k}}(\vec{r}; r \rightarrow \infty) \rightarrow A \left[e^{i\vec{k} \cdot \vec{r}} + \frac{f(\hat{\Omega})}{r} e^{i\delta} \right]$$
- The incident wave function is:

$$\psi_{inc}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} = e^{ikr \cos \theta} = e^{i\rho \mu}$$
 with $\rho = kr$ & $\mu = \cos \theta$
- The expansion of the incident wave function in terms of spherical harmonics and Bessel functions is:

$$e^{i\vec{k} \cdot \vec{r}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} c_{l,m} Y_l^m(\hat{r}) j_l(\rho) = \sum_{l=0}^{\infty} a_l P_l(\cos \theta) j_l(\rho)$$
- The expansion of the incident wave function in terms of Legendre polynomials and Bessel functions is:

$$e^{i\rho \mu} = \sum_{l=0}^{\infty} a_l P_l(\mu) j_l(\rho)$$
- The scattering amplitude a_l is circled in pink, with a question mark next to it: $a_l = ?$
- The NPTEL logo is in the bottom left corner.
- The text "PCD STITACS Unit 1 Quantum Theory of Collisions" is at the bottom center.
- The number "9" is in the bottom right corner.

So we know that the full solution will consist of the incident wave plus a scattered wave which will be a spherically outgoing wave. So, it will have e to the ikr its size will diminish as 1 over r because the intensity of the wave will go as 1 over r square. And the area of the sphere which is expanding from the target center also increases as r square okay.

Area of a sphere goes as r square, so one over r takes care of the size of the scattered beam. In addition to that there will be a certain angle dependent modulation of this amplitude. This is the scattering amplitude and as you can see this scattering amplitude which is dependent on an angle.

So, omega is a unit vector which gives the direction of scattering and this f of omega you can see already from this equation must have the dimensions of length because you have the 1 over length over here, 1 over r and then together with this e to the ikr you must have a dimensionless quantity here okay.

So, f of omega the scattering amplitude will necessarily have the dimensions of length the incident wave is e to the ik dot r and you would have discussed these things in your earlier

course in quantum mechanics or atomic physics. So, I will spend a few minutes very quickly recapitulate the essential results. So, that we build our vocabulary to discuss the scattering process okay.

So the incident wave is $e^{i\mathbf{k} \cdot \mathbf{r}}$ which I can write as $e^{i\rho \cos \theta}$ and I can introduce for simplicity the variables ρ and μ , μ being $\cos \theta$ and ρ mean kr and then expand $e^{i\rho \mu}$ in terms of the Legendre polynomials functions of the angles functions of cosine theta and the distance dependence being given by the spherical Bessel functions j_l okay.

Now this is basically an expansion in spherical harmonics but because of the azimuthal symmetry the essential dependence is on the angle theta. So, you have these coefficients a_l which will take care of that okay. So, a_l are the unknowns which we have to find, we know the Bessel functions, we know the Legendre polynomials, we want to find out what the coefficients a_l are okay.

They are the ones which will determine the mix how much of $P_l(\mu)$ and the corresponding spherical Bessel function $j_l(\rho)$ contribute to the incident plane wave that is determined by the coefficient a_l .

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The slide contains the following mathematical derivation:

$$e^{i\rho\mu} = \sum_{l=0}^{\infty} a_l P_l(\mu) j_l(\rho)$$

$$\int_{-1}^{+1} e^{i\rho\mu} P_{l'}(\mu) d\mu = \sum_{l=0}^{\infty} a_l \left[\int_{-1}^{+1} P_l(\mu) P_{l'}(\mu) d\mu \right] j_l(\rho)$$

$$= \sum_{l=0}^{\infty} a_l \left[\frac{2}{2l+1} \delta_{ll'} \right] j_l(\rho) \quad \text{Orthogonality of the Legendre polynomials}$$

$$= a_{l'} \left[\frac{2}{2l'+1} \right] j_{l'}(\rho)$$

Dropping the redundant 'prime'

$$\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu) d\mu = a_l \left[\frac{2}{2l+1} \right] j_l(\rho)$$

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So, we can determine this a_l quite easily by using the orthogonality properties of the Legendre polynomials because we know that if you integrate. If you multiply the left-hand side by a Legendre polynomial and integrate over the range of cosine theta okay which goes from -1 to +1 then because of the orthogonality of these two Legendre polynomials those with different l indices orthogonal to each other. So, there is a Kronecker delta, $\delta_{ll'}$

and using this orthogonality of the legendary polynomial this summation over l contracts and you get a single term.

And now you really do not need the prime anymore because only one l value has survived. So, we can drop the prime and we have this orthogonality relation that the integral over this entire range of cosine theta is equal to al times 2 over 2l + 1 times the spherical Bessel function and this tells us that we can get al from everything else that is there in this equation okay.

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The slide contains the following mathematical content:

$$\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu) d\mu = a_l \left[\frac{2}{2l+1} \right] j_l(\rho)$$

$$\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu) d\mu = \int_{-1}^{+1} \overset{1^{st} \text{ function}}{P_l(\mu)} \overset{2^{nd} \text{ function}}{e^{i\rho\mu}} d\mu$$

Integral of a product of two functions

$$= \left[P_l(\mu) \frac{e^{i\rho\mu}}{i\rho} \right]_{-1}^{+1} - \int_{-1}^{+1} P_l'(\mu) \frac{e^{i\rho\mu}}{i\rho} d\mu$$

$P_l'(\mu) = \frac{d}{d\mu} P_l(\mu)$

$$\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu) d\mu = \frac{P_l(\mu=1)e^{i\rho}}{i\rho} - \frac{P_l(\mu=-1)e^{-i\rho}}{i\rho} - \frac{1}{i\rho} \int_{-1}^{+1} P_l'(\mu) e^{i\rho\mu} d\mu$$

$P_l(\mu=1) = 1$

$P_l(\mu=-1) = (-1)^l P_l(\mu=1) = (-1)^l$

$$\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu) d\mu = \frac{e^{i\rho} - (-1)^l e^{-i\rho}}{i\rho} - \frac{1}{i\rho} \int_{-1}^{+1} P_l'(\mu) e^{i\rho\mu} d\mu$$

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So, all we need to do is to evaluate this integral and get al in terms of that, that is our question. So, how do we do that we evaluate this integral this is an integral of a product of two functions the first function is let us say the Legendre polynomial the second function is e to the i Rho mu. So you just evaluate this integral which is the product of two functions.

So, you get these two terms and over here you get the integral of the differential of the first function times the integral of the second okay. So, this is the result you get from the integration of a product of two functions. And over here there are two terms one corresponding to mu = +1 from which you must subtract the value of this term corresponding to mu = -1.

So let us do that explicitly so this is the term corresponding to mu = +1 and then from this you subtract there is a minus sign here the term corresponding to mu = -1 and then you have got this integral coming over here and what is Pl at mu = 1, it is always equal to 1 no matter what l is and what is Pl at mu = -1 no matter what l is, it is always -1 to the power l. So, we know these values explicitly.

So, we can plug in these values and you now have this integral to be equal to e to the i Rho coming from here minus which is this sign, -1 to the l which is coming from this, e to the -i Rho and then you have this i Rho in the denominator and then you have the integral which is left over.

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$$\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu) d\mu = \frac{e^{i\rho} - (-1)^l e^{-i\rho}}{i\rho} - \frac{1}{i\rho} \int_{-1}^{+1} P_l'(\mu) e^{i\rho\mu} d\mu$$

$$\Rightarrow \int_{-1}^{+1} e^{i\rho\mu} P_l(\mu) d\mu = \frac{e^{i\rho} - (-1)^l e^{-i\rho}}{i\rho} + O(\rho^2)$$

we had: $\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu) d\mu = a_l \left[\frac{2}{2l+1} \right] j_l(\rho)$ as $\rho \rightarrow \infty$

$$a_l \left[\frac{2}{2l+1} \right] j_l(\rho) = \frac{e^{i\rho} - (-1)^l e^{-i\rho}}{i\rho}$$

$$e^{i\pi} = (e^{i\pi})^l = (-1)^l$$

$$a_l \left[\frac{2}{2l+1} \right] j_l(\rho) = \frac{e^{i\rho} - e^{i\pi l} e^{-i\rho}}{i\rho}$$


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So, this is your result and this you can integrate further again as a product of two functions and every time you will get an extra 1 over Rho term okay. So, it is, it will be of the order of 1 over Rho squared and in the asymptotic region as Rho tends to infinity as r tends to infinity because Rho is kr as r tends to infinity that is where you keep the detector okay, well away from the scattering zone.

So, your interest is in the asymptotic region and in this domain you can ignore the 1 over Rho square terms and you are left with only the first term which gives you this value of the integral and now you had earlier this integral to be given by a_l times $\frac{2}{2l+1}$ times the spherical Bessel function the left hand sides are the same so the right hand sides better be the same you equate the two right-hand sides okay.

And now you get a_l in terms of the rest of it because you know what j is okay. So, knowing j you can find what a_l is. And what is j , j is the spherical Bessel functions so you can put its value at any value of Rho and get this here. Now it is convenient to write this -1 to the l as e to the $il\pi$, because you know that e to the $il\pi$ is the l th power of e to the $i\pi$, which is -1 to the power l . So, instead of -1 to the l it is convenient to write this as e to the $il\pi$ okay.

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$$a_l \left[\frac{2}{2l+1} \right] j_l(\rho) = \frac{e^{i\rho} - e^{i\pi} e^{-i\rho}}{i\rho}$$

$$a_l \left[\frac{2}{2l+1} \right] j_l(\rho) = \left[\frac{e^{i\rho} - e^{i\frac{\pi}{2}} e^{i\frac{\pi}{2}} e^{-i\rho}}{i\rho} \right]$$

$$a_l \left[\frac{2}{2l+1} \right] j_l(\rho) = e^{i\frac{\pi}{2}} \left[\frac{e^{i\rho} e^{-i\frac{\pi}{2}} - e^{-i\frac{\pi}{2}} e^{-i\rho}}{i\rho} \right]$$

$$a_l \left[\frac{2}{2l+1} \right] j_l(\rho) = i^l \left[\frac{e^{i(\rho - \frac{l\pi}{2})} - e^{-i(\rho - \frac{l\pi}{2})}}{i\rho} \right] = i^l \left[\frac{2i \sin\left(\rho - \frac{l\pi}{2}\right)}{i\rho} \right]$$

$$e^{i\pi} = (e^{i\pi})^l = (-1)^l$$

$$= (i^2)^l = i^{2l}$$

$$e^{i\frac{\pi}{2}} = \left(e^{i\frac{\pi}{2}} \right)^l = i^l$$

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And furthermore it is convenient to break this $e^{i\pi}$ into two pieces $e^{i\frac{\pi}{2}}$ times $e^{i\frac{\pi}{2}}$, because that allows you to extract one of these $e^{i\frac{\pi}{2}}$ as a common factor so you pull out $e^{i\frac{\pi}{2}}$ as a common factor but it was not there over here.

So, this phase must drop by $e^{-i\frac{\pi}{2}}$ and you are left with only one of these two factors in the second term. So it is very convenient to write the phases in this particular form and furthermore to recognize that this $e^{i\frac{\pi}{2}}$ is the same as i to the power l . So, since $e^{i\frac{\pi}{2}}$ is the same as i to the power l , I replace this $e^{i\frac{\pi}{2}}$ by i to the power l .

But the one inside I leave them alone okay as in the previous step and this allows me to write these two exponential terms in a very similar form. One with a $+$ sign this is $e^{i(\rho - \frac{l\pi}{2})}$ whereas this is $e^{-i(\rho - \frac{l\pi}{2})}$ and these two terms together give you this twice i sinusoidal term okay. So, you can write it in terms of the sinusoidal function instead of the exponential form.

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$$a_l \left[\frac{2}{2l+1} \right] j_l(\rho) = i^l \left[\frac{e^{i(\rho - \frac{l\pi}{2})} - e^{-i(\rho - \frac{l\pi}{2})}}{i\rho} \right]$$


$$a_l \left[\frac{2}{2l+1} \right] j_l(\rho) = i^l \left[\frac{2i \sin\left(\rho - \frac{l\pi}{2}\right)}{i\rho} \right]$$

Now, $j_l(\rho) \underset{\rho \rightarrow \infty}{=} \frac{\sin\left(\rho - \frac{l\pi}{2}\right)}{\rho} \Rightarrow a_l = i^l (2l+1)$

$e^{i\rho\mu} = \sum_{l=0}^{\infty} a_l P_l(\mu) j_l(\rho)$ We got a_l from $\rho \rightarrow \infty$, but it is valid for all ρ since $a_l \neq f(\rho)$.

$$\Rightarrow e^{i\rho\mu} = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\mu) j_l(\rho)$$

i.e. $e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) j_l(kr)$



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So this is just a rearrangement of terms which gives us a very convenient form of writing these expressions and now you have a which can be written in terms of the sinusoidal function but you already know that the spherical Bessel function, you can evaluate this from any value of Rho the easiest one is the asymptotic value because that is well known and it does not matter at what value of Rho do you determine this.

Because it is applicable to the entire range Rho going from 0 through infinity so you might as well evaluate it for the easiest one which is Rho tending to infinity and the spherical Bessel function as Rho tends to infinity is the sign Rho - l pi by 2 divided by Rho and that tells us that al is given by i to the l 2l+1 and we have evaluated it for the asymptotic region by of course it is valid for the entire range because it is independent of Rho right.

So we now have al and writing this al explicitly as i to the power l 2l + 1 we have got the incident wave described as such. So this is in terms of the Legendre polynomials and the spherical Bessel functions. You can write it in terms of kr cos theta as well. (Refer Slide Time: 33:55)

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) j_l(kr) \quad \theta = \angle(\hat{k}_i, \hat{r})$$

Spherical harmonics addition theorem (Unit 2, STiAP slide 94) <http://nptel.iitm.ac.in/courses/115106057/9>

$$P_\ell(\hat{u}\cdot\hat{v}) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_{\ell m}^*(\hat{v}) Y_{\ell m}(\hat{u})$$

$$e^{i\hat{k}_i\cdot\hat{r}} = 4\pi \sum_{l=0}^{\infty} i^l j_l(kr) \left[\sum_{m=-\ell}^{\ell} Y_{\ell m}^*(\hat{k}_i) Y_{\ell m}(\hat{e}_r) \right]$$

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Again using the addition theorem for spherical harmonics you can write this equivalently in this form. And I would like you to be referred to this particular link in which the equivalence of these two forms is established using the addition theorem for spherical harmonic. So, I will not work out those details now all right. (Refer Slide Time: 34:26)

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

$$\psi_{inc}(\vec{r}; r \rightarrow \infty) \rightarrow \sum_l i^l (2l+1) P_l(\cos\theta) \frac{\sin(kr - \frac{l\pi}{2})}{kr}$$

$$\psi_{inc}(\vec{r}) \rightarrow \sum_l i^l (2l+1) P_l(\cos\theta) \frac{e^{i(kr - \frac{l\pi}{2})} - e^{-i(kr - \frac{l\pi}{2})}}{2ikr}$$

$$e^{\frac{l\pi}{2}} = \left(e^{\frac{i\pi}{2}} \right)^l = i^l$$

$$\psi_{inc}(\vec{r}) \rightarrow \sum_l (2l+1) P_l(\cos\theta) \frac{e^{ikr} - e^{-ikr} e^{+\frac{l\pi}{2}} e^{+\frac{l\pi}{2}}}{2ikr}$$

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So now we know that this incident wave has got this asymptotic form okay. You can write it in terms of the sinusoidal functions or in terms of the exponential functions they are both equivalent. And you can again exploit the fact that e to the il pi by 2 is given by i to the l, so you can write this i to the l as e to the il pi by 2 and you can multiply this throughout.

So, in the first term you get e to the ikr because there is an e to the -il pi by 2 which is multiplied by i to the l which is e to the il pi by 2. So, together they will give you unity, so you get e to the ikr and then you have this term so these are equivalent forms in which you will find these relations.

(Refer Slide Time: 35:27)

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

$$\psi_{inc}(\vec{r}) \xrightarrow{r \rightarrow \infty} \sum_l (2l+1) P_l(\cos \theta) \frac{e^{i\vec{k}\cdot\vec{r}} - e^{-i\vec{k}\cdot\vec{r}} e^{i\frac{l\pi}{2}} e^{i\frac{l\pi}{2}}}{2ikr}$$

$$\psi_{inc}(\vec{r}) \xrightarrow{r \rightarrow \infty} \sum_l (2l+1) P_l(\cos \theta) \frac{e^{i\vec{k}\cdot\vec{r}} - e^{-i\vec{k}\cdot\vec{r}} (-1)^l}{2ikr}$$

$$\psi_{inc} \xrightarrow{r \rightarrow \infty} \frac{1}{2ikr} \sum_l (2l+1) \left[P_l(\cos \theta) e^{i\vec{k}\cdot\vec{r}} - P_l(\cos \theta) (-1)^l e^{-i\vec{k}\cdot\vec{r}} \right]$$

$$\psi_{inc} \xrightarrow{r \rightarrow \infty} \frac{1}{2ikr} \sum_l (2l+1) \left[P_l(\cos \theta) e^{i\vec{k}\cdot\vec{r}} - P_l(-\cos \theta) e^{-i\vec{k}\cdot\vec{r}} \right]$$

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So, you get $e^{i\pi}$ over here because of these two factors which is -1 to the l and because you have -1 to the l over here if you multiply this term and this term both terms by $P_l \cos \theta$ you get $P_l \cos \theta$ times $e^{i\vec{k}\cdot\vec{r}}$ in the first term and in the second term you have got $P_l \cos \theta (-1)^l$ and then $e^{-i\vec{k}\cdot\vec{r}}$.

But then you can combine these two terms because $P_l \cos \theta (-1)^l$ is nothing but $P_l(-\cos \theta)$ okay. So, we use these identities and we have got this relationship for the incident plane wave.

(Refer Slide Time: 36:23)

$$e^{i\vec{k}\cdot\vec{r}} \xrightarrow{r \rightarrow \infty} \frac{1}{2ikr} \sum_l (2l+1) \left[P_l(\cos \theta) e^{i\vec{k}\cdot\vec{r}} - P_l(-\cos \theta) e^{-i\vec{k}\cdot\vec{r}} \right]$$

What will be the result of scattering by a potential?

$$\psi_{tot}(\vec{r}) \xrightarrow{r \rightarrow \infty} \frac{1}{2ikr} \sum_l c_l (2l+1) \left[P_l(\cos \theta) e^{i(kr + \delta_l)} - P_l(-\cos \theta) e^{-i(kr + \delta_l)} \right]$$

δ_l : phase shift of the l^{th} partial wave

condition:
 for potentials that fall
 faster than the *Coulomb* potential, i.e. faster than $\frac{1}{r}$ as $r \rightarrow \infty$.

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Very good now you have the incident plane wave exactly and the question is how is it going to be affected by scattering okay. So, when there is a scattering potential the solution will have a very similar form. The total wave function will be given by almost the same form except for a phase shift which is caused by the scattering potential okay.

That is the only thing it is going to change and then it will change the mix of the various partial waves okay. For each l , l is a orbital angular momentum quantum number which goes from 0 to infinity. Each value of l corresponds to 1 partial wave and what is the contribution of these terms corresponding to each that is determined by this mixing coefficient which is c_l . So, this is the unknown now okay.

This will also determine the size of the total wave function because it is multiplying this whole thing. So, the amplitude is going to be determined by the mixing factors c_l , so it is a part of the normalization and what the scattering potential does is to introduce these phase shifts δ_l for each l th partial wave that is the only thing this scattering does okay.

Now there is a certain condition yes, yeah this you have got the incident plane wave here and we are asking the question in what way is the solution to the Schrodinger equation going to be different when you insert the target if there was no target all you have is the incident beam and we have described it, if you now have a target which will interact with the incident beam resulting in scattering.

The net wave function has exactly the same form. So, you have got a summation over l in both cases. You got a $1/2$ in both cases; you have got each partial wave scaled by $2l+1$ in both cases. There is a $2l+1$ factor here; there is a $2l+1$ factor here as well. Then it is a superposition of these two terms, each term is a product of the legendary polynomial and an exponential function which is a spherical outgoing wave.

And this is a spherical in going way so $e^{i kr}$ is the spherically outgoing wave and you know why it is an outgoing wave and $e^{-i kr}$ is a spherically in going wave and again you know why it is an in going wave. So it is a mix of an outgoing wave and in going wave okay. But what is the phase of this outgoing wave and in going wave? Now this phase is not the same as it was for the free incident beam.

This phase is shifted by the scattering interaction. Now this is a very general result it expresses the result of scattering for any scattering phenomenon nevertheless subject to certain conditions and the condition which holds; which must be satisfied for us to be able to write the scattering potential, the result of the scattering potential in this form is that the scattering potential must fall faster than the Coulomb potential that is the condition.

Every physical potential will fall as you go away from it okay because the physical influence of anything will reduce with distance. So, we know that it is going to become weaker and weaker but at what rate does it get weaker does it go become weaker as $1/r$ or as $1/r^2$

squared or some function of 1 over r + 1 over r squared or some polynomial 1 over r + a times 1 over r + b times 1 over r squared + c times, 1 over r cube okay.

All of this the effective rate at which it falls must be faster than 1 over r . If it does not meet this condition then the phase shift is not given by this but simple form. You have to do the analysis in a slightly different way but for those potentials which following faster than the Coulomb potential this is the form of the total wave function.

(Refer Slide Time: 41:27)

The slide contains the following mathematical expressions and a diagram:

$$e^{ikz} \xrightarrow{r \rightarrow \infty} \frac{1}{2ikr} \sum_l (2l+1) [P_l(\cos\theta)e^{ikr} - P_l(-\cos\theta)e^{-ikr}]$$

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

The diagram shows a blue arrow representing an incident plane wave hitting a red circular target. Scattered waves are shown as blue arrows radiating outwards from the target.

δ_l : phase shift of the l^{th} partial wave

$$\psi_{\text{Tot}}(\vec{r}) \xrightarrow{r \rightarrow \infty} \frac{1}{2ikr} \sum_l c_l (2l+1) [P_l(\cos\theta)e^{i(kr+\delta_l)} - P_l(-\cos\theta)e^{-i(kr+\delta_l)}]$$

Please refer to details from :
 PCD STIAP 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%28%29%30)
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NPTEL logo and page number 19 are also present.

And we have discussed this in an earlier course and the derivation for this particular result is available in this lecture which is also available at this link. So, if you look at lecture number 27, 28, 29 and 30 in this particular course special topics in atomic physics from unit 6 the complete derivation for why this potential must fall faster than the Coulomb potential is available there.

So, I will not repeat that discussion over here okay. So, for those potentials which fall faster than the Coulomb potential the condition being explained in these earlier lectures which you can easily find on the internet? The total wave function has got a similar form to the incident plane wave with the difference that the scattering phase shift is introduced and this scattering phase shift gives us information about the target potential.

(Refer Slide Time: 42:38)

$$\psi_{Tot}(\vec{r}) \xrightarrow{r \rightarrow \infty}$$

$$\frac{1}{2ikr} \sum_l c_l (2l+1) \left[P_l(\cos\theta) e^{i(kr+\delta_l)} - P_l(-\cos\theta) e^{-i(kr+\delta_l)} \right]$$

choice of normalization

c_l depends on the boundary conditions

Please refer to details from : PCD STIAP Unit 6 Probing the Atom

$c_l = e^{\pm i\delta_l}$

Lecture link: <http://nptel.iitm.ac.in/courses/115106057/27> & /28 & /29 & /30

$\psi_{Tot}^+(\vec{r}, t) \rightarrow$ outgoing wave boundary conditions
 $\psi_{Tot}^-(\vec{r}, t) \rightarrow$ ingoing wave boundary conditions

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So these details are from the unit 6 of this other course whose lectures are available and let me also remind you that c_l over here which is the mixing coefficient for each l th partial wave is going to determine the normalization and how is this normalization done okay. So this must be done according to the boundary conditions okay.

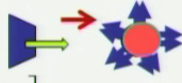
So, the boundary conditions are important because you have two different kinds of boundary conditions when you deal with a scattering experiment. One what are known as the outgoing wave boundary conditions and the other which are known as in going way boundary conditions? So if you have the outgoing wave boundary conditions then c_l is $e^{i\delta_l}$, if you have the ingoing way boundary conditions you have $c_l = -i\delta_l$.

And with reference to these different boundary conditions you have got the solutions either with a plus superscript sign or a minus superscript sign over here corresponding to the outgoing wave boundary conditions or in going way boundary conditions and these boundary conditions are involved for different kind of scattering situations.

One in quantum collisions you have got the outgoing wave boundary conditions but if you are using this analysis to describe a photo ionization event you would use the ingoing wave boundary conditions. And again I will not repeat these details because they are available in unit 6 of the course special topics in atomic physics and I will refer you to lecture number 27, 28, 29 and 30.

Where these boundary conditions are discussed in detail I will urge you to recapitulate those results. So, that when we go for the next class you will have it at the top of your mind and with these boundary conditions you have the scattering solution.
(Refer Slide Time: 44:49)

Outgoing wave boundary condition

$\hat{k}_i = \hat{e}_z$ 


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

$c_l = e^{i\delta_l}$ gives: scattering amplitude

$$f(k, \theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [e^{2i\delta_l(k)} - 1] P_l(\cos \theta)$$

Faxen-Holtzmark's formalism

Each l^{th} term gives the contribution of the l^{th} partial wave to the scattering amplitude.

 Reference: Quantum Theory of Collisions by Charles J Joachain North-Holland Publishing Co. // Section 3.2 // see Eq.3.27, page 49
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Our focus in this unit is on quantum collisions so we will employ the outgoing wave boundary conditions. So, you have got a spherical outgoing wave in the final state and the scattering amplitude is what we want to determine because it is going to tell us how much of the outgoing wave scattered wave is mixed with the incident wave into the total wave function right.

So, that is the main object of interest and the target of our analysis this scattering amplitude we already know will have the dimensions of length. And again from the details of the discussion that we have had in the core special topics and atomic physics this sketching amplitude is given by the Faxen and Holtzmark's formalism.

In which the f it is dependent on energy and therefore on momentum as well as on the angle theta and it is given by this infinite sum out of which typically only the first few terms contribute because of the centrifugal barrier effect which we have discussed earlier okay. (Refer Slide Time: 46:06)

$\psi_{Tot}^+(\vec{r}, t) \Big|_{r \rightarrow \infty} \rightarrow$

$$e^{+i(kz-ot)} + \frac{e^{+i(kr-ot)}}{r} \left\{ \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [e^{2i\delta_l(k)} - 1] P_l(\cos \theta) \right\}$$
 $C_l = e^{i\delta_l(k)}$ describes 'collisions'

$\psi_{Tot}^-(\vec{r}, t) \Big|_{r \rightarrow \infty} \rightarrow$

$$e^{+i(kz+ot)} + \frac{e^{+i(kr+ot)}}{r} \left\{ \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [e^{2i\delta_l(k)} - 1] P_l(\cos \theta) \right\}$$
 $C_l = e^{-i\delta_l(k)}$ describes 'photoionization'

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So, you have got infinite turns over here and these details again I will not discuss in this course they have been discussed in unit 6 of the course which is available and you use the outgoing wave boundary conditions for quantum collisions the ingoing way boundary conditions e to the -i delta l for photo ionization. In which case you have got a different final state which you must use in photo ionization analysis.

And then you get, if you look at the complete time evolution you get a picture that the scatterer sends out Spherical outgoing waves in the scattering experiment. Whereas in the photo ionization experiment because of in going way boundary conditions you have got the photoelectron which is ejected along a unique escape channel okay.

So, there is a unique escape channel for the photoelectron. So again these things will not be discussed in details but you can access this information in the previous course which is available.

(Refer Slide Time: 47:10)

Θ : operator for TIME REVERSAL SYMMETRY

$\psi_{Tot}^+(\vec{r}, t) \Big|_{r \rightarrow \infty} \rightarrow$

$$e^{+i(kz-ot)} + \frac{e^{+i(kr-ot)}}{r} \left\{ \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [e^{2i\delta_l(k)} - 1] P_l(\cos \theta) \right\}$$

Θ [collision] = photoionization

$\psi_{Tot}^-(\vec{r}, t) \Big|_{r \rightarrow \infty} \rightarrow$

$$e^{+i(kz+ot)} + \frac{e^{+i(kr+ot)}}{r} \left\{ \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [e^{2i\delta_l(k)} - 1] P_l(\cos \theta) \right\}$$

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So these two processes the outgoing wave boundary conditions and the ingoing way boundary conditions they are described by the same quantum mechanics. They are related to each other by the time reversal symmetry. This is part of the detailed discussion in the previous course.

So, I will refer you to those lectures and the time reversal symmetry connects the solutions corresponding to quantum collisions with the solutions corresponding to photo ionization the connection being the boundary condition you employ the outgoing wave boundary condition in one case and the ingoing way boundary condition in the other okay.

(Refer Slide Time: 48:05)

$C_l = e^{i\delta_l(k)}$
 'collisions'
 $\psi_{\vec{k}_i}^{(+)}(\vec{r}; r \rightarrow \infty) \xrightarrow{r \rightarrow \infty} A(k) \left[e^{i\vec{k}_i \cdot \vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr} \right]$
 $f(k, \theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [e^{2i\delta_l(k)} - 1] P_l(\cos \theta)$
 Contributions of Faxen-Holtzmark's formalism the partial waves to the scattering amplitude.
 QUESTIONS?
 Write to: pcd@physics.iitm.ac.in
 Next class: OPTICAL THEOREM
 Reference: Quantum Theory of Collisions by Charles J Joachain North-Holland Publishing Co. // Section 3.2 // see Eq.3.27, page 49
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So, please recapitulate these boundary conditions and our result today is that we have got an expression for the scattering amplitude given by the Faxen and Holtzmark's equation okay. This is what gives us the contributions of the partial waves to the scattering amplitude and with that I will conclude today's class.

What we will do in the next class is discuss a very famous here in scattering theory which is known as the optical theorem. If there are any questions I will be happy to take otherwise goodbye for today.