

Select/Special Topics in Atomic Physics
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Lecture - 28
 Atomic Probe: Collisions and Spectroscopy
 Scattering Phase Shifts and Boundary Conditions

Greetings, so we will discuss Scattering Phase Shifts and how they are related to the Boundary Conditions and also to the normalization of the wave function.

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‘free particle’ as special case of spherically symmetric potential
 $\left\{ \text{ignoring } \frac{1}{r^2} \right\}_{r \rightarrow \infty}$
 $R_{kl}(r \rightarrow \infty) \underset{\text{asymptotic behavior}}{\approx} \frac{N_l(k) \sin\left(kr - l\frac{\pi}{2}\right)}{r}$
 $E > 0$ continuum for $V = 0$

for $V(r) \neq 0$ Scattering phase shift $\delta_l(k)$ due to the target potential
 $R_{cl}(r) \xrightarrow{r \rightarrow \infty} A_l(k) \frac{\sin\left(kr - \frac{l\pi}{2} + \delta_l(k)\right)}{r}$


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So, we have seen that free particle solution has got the general form the l 'th solution for l quantum number, when the potential is 0 which is the case of free particle as a special case of spherically symmetric potential. And this is the general solution, now if V is not really equal to 0, you really have a scattering potential which is the case of interest, then the solution is exactly like this, it is sinusoidal function with 1 over r in the denominator. The argument is $kr - l\pi/2$ in both cases, except that in this case when V is not equal to 0, there is additional space shift. And this space shift is scattering space shift which contains information about the potential.

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$E > 0$ continuum

$$R'' + \frac{2}{r} R' - \frac{l(l+1)}{r^2} R + \frac{2\mu}{\hbar^2} [E - V(r)] R = 0$$

$$R_d(r) = \frac{y_d(r)}{r}; \quad \text{i.e. } y_d(r) = r R_d(r)$$


$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \left\{ V(r) + \frac{1}{2m} \frac{l(l+1)}{r^2} \right\} - E \right] y_d(r) = 0$$

$$\left[\frac{d^2}{dr^2} + k^2 - U(r) - \frac{l(l+1)}{r^2} \right] y_l(k, r) = 0 \quad U(r) = \frac{2mV(r)}{\hbar^2}$$

$V(r)$ We now discuss how

$V(|\vec{r}|) \neq 0$ produces the phase shift $\delta_l(k)$

$r = a \quad V(r > a) \rightarrow \text{"weak"} = ? \quad r$

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So, let us have a look at this problem and we look only at the radial part because the angle of the solution we already know those are the spherical harmonics. And we set up this differential equation for y , where y over r is radial function, so with this choice y will need to satisfy differential equation, which is given over here. And if you remove these constants by defining the potentials twice and V over \hbar cross square, you can write it in a way which is rather simple and concise.

So, that you do not have to write too many constants needlessly, and we will now discuss how the potential V r produces the pressure that is the result that we made use of in the previous class, that the scattering potential generates a space shift. Today initially we will first demonstrate, how the scattering phase shifts generate the potential, so the potential that we are going to look at is of this form, that as r turns to infinity any physical potential, will have you know an influence which will become weaker and weaker as you go farther away from the center of the potential.

So, as turns to infinity in the asymptotic region the potential will become very weak, and we presume that no matter what is the detailed structure of the scattering potential, in the problem of our interest. It is weak enough in the asymptotic region that is a fairly acceptable assumption, we nevertheless have to discuss by weak what exactly do you mean is 1 over r weak enough is 1 over r square weak or is 1 over r cube weak these are all weak potentials.

They all go to 0 as r is equal to infinity right, 1 over r cube also goes to 0, 1 over r square also goes to 0, 1 over r also goes to 0. So, all are these case admissible in our treatment the answer is no, and what exactly is this restriction is what I am going to discuss now. So, we will answer this question as to what we mean by the potential being weak in the asymptotic region.

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The slide contains the following content:

- A graph of $V(r)$ versus r . The potential is zero for $r > a$, which is labeled as "weak".
- The differential equation:
$$\left[\frac{d^2}{dr^2} + k^2 - U(r) - \frac{l(l+1)}{r^2} \right] y_l(k, r) = 0 \quad U(r) = \frac{2mV(r)}{\hbar^2}$$
- For large r , the potential is "weak", leading to the solution: $y_l(k, r) = F_l(k, r) e^{\pm ikr}$
- $F_l(k, r)$ would be constant if the potential were zero.
- Our case \rightarrow
- $\rightarrow F_l(k, r)$: rather slowly varying function of r
- The differential equation becomes:
$$\left[\frac{d^2}{dr^2} + k^2 - U_l^*(r) \right] y_l(k, r) = 0 \quad \text{where } U_l^{\text{effective}}(r) = U(r) + \frac{l(l+1)}{r^2}$$

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So, this is the form of the differential equation that y must satisfy, and assuming that this potential is weak, and we will define what is meant by weakness. The solution will be given by this exponential function multiplied by some other r dependant function, which is represented here by capital F , if this potential was weak enough, so weak that you can simply pretend that it is not there it is 0. Then you have the case of free particle right, and in that case the entire r dependence would be contain in the exponential function e to the plus or minus $i k r$ would be the exact solution, with this potential vanishing.

The exact solution would be given by e to the plus or minus $i k r$, but when this is not completely 0, but only weak. Then the function F would not be a constant, it could depend on r , but it could only be weakly depend on r , so now, we know that when we are dealing with a weak potential. A potential that is weak in the asymptotic region as r tends to infinity, the solution would be given by this exponential function multiplied by a factor, which is not a constant.

It does depend on r all the r dependencies extracted in the e to the $i k r$ function, but the residual r dependence is packed in this function F , which is not quite a constant. But, it is not very strongly dependent on r which means r changes the function would change, but not very rapidly, but rather weakly right. If it is completely independent of r it would be flat, if you plot it as a function of r it would just be a horizontal line that is a function that does not depend on r .

If it depends strongly on r it would have very many wiggles ups and downs, if it is only weakly dependent on r , it will have very gentle ripples over a constant line that is what is meant by weakly dependent function. So, F is a weakly dependent function of r , it would. In fact, be a constant if the potential were 0 and this is the case that we are considering. So, now, we know something about the function F that it is a weakly dependent it does depend on r , but only weakly, so.

And, I put the two potentials there is this real physical potential U which is coming from real physical potential V , so other than this scale factors $2m$ over \hbar^2 cross square. So, U is the real physical potential, l into $l(l+1)$ over r^2 is the centrifugal potential, which has come from a reduction of three dimensional problem to the one dimensional problem. So, the one dimensional effective potential is U plus $l(l+1)$ by r^2 this is the effective potential. And this is the differential equation that we want to solve, what we do know that y can be written as a product of these two functions, and you can take the derivative of y as a product of these two functions of r .

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$$\left[\frac{d^2}{dr^2} + k^2 - U_l^e(r) \right] y_l(k, r) = 0 \quad \text{where } U_l^{\text{effective}}(r) = U(r) + \frac{l(l+1)}{r^2}$$

$$y_l(k, r) = F_l(k, r)e^{\pm ikr} \quad \text{slowly varying function of } r$$

$$y_l'(k, r) = \pm i k F_l(k, r)e^{\pm ikr} + F_l'(k, r)e^{\pm ikr}$$

$$y_l''(k, r) = (\pm i k)^2 F_l(k, r)e^{\pm ikr} \pm i k F_l'(k, r)e^{\pm ikr} + F_l''(k, r)e^{\pm ikr} + i k F_l'(k, r)e^{\pm ikr}$$

$$y_l''(k, r) = (\pm i k)^2 F_l(k, r)e^{\pm ikr} \pm 2 i k F_l'(k, r)e^{\pm ikr} + F_l''(k, r)e^{\pm ikr} + F_l(k, r)e^{\pm ikr} [k^2 - U_l^e(r)] = 0$$

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So, this is what we have got F is a slowly or slowly varying function of r , so you can take its first derivative, which is the derivative of product of these two functions. So, it is plus or minus $i k F$ times e to the plus or minus $i k r$ right, and then you have the derivative of F . Similarly you take the second derivative, and you have two terms which are similar, so you can add them together and after adding these two terms you have got plus or minus twice $i k F$ prime. And this is and these are three terms that you get for your y double prime. So, now you have got your function y expressed in terms of F you have y prime, and you also have y double prime. And you can put all of them in this differential equation.

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$$\left[\frac{d^2}{dr^2} + k^2 - U_l^e(r) \right] y_l(k, r) = 0 \quad \text{where } U_l^{\text{effective}}(r) = U(r) + \frac{l(l+1)}{r^2}$$

$$y_l(k, r) = F_l(k, r)e^{\pm ikr} \quad y_l'(k, r) = \pm i k F_l(k, r)e^{\pm ikr} + F_l'(k, r)e^{\pm ikr}$$

$$y_l''(k, r) = (\pm i k)^2 F_l(k, r)e^{\pm ikr} \pm 2 i k F_l'(k, r)e^{\pm ikr} + F_l''(k, r)e^{\pm ikr} + F_l(k, r)e^{\pm ikr} [k^2 - U_l^e(r)] = 0$$

$$\left[(\pm i k)^2 F_l(k, r)e^{\pm ikr} \pm 2 i k F_l'(k, r)e^{\pm ikr} + F_l''(k, r)e^{\pm ikr} + F_l(k, r)e^{\pm ikr} [k^2 - U_l^e(r)] \right] = 0$$

$$F_l''(k, r) \pm 2 i k F_l'(k, r) - U_l^e(r) F_l(k, r) = 0$$

$$\frac{F_l''(k, r)}{F_l(k, r)} \pm 2 i k \frac{F_l'(k, r)}{F_l(k, r)} = U_l^e(r)$$

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So, let us do that this is the differential equation, you have got y , you have got y prime and you got y double prime, And when you put them all together in this differential equation, you will discover that F must satisfy a differential equation, in which you have put all of these terms right. So, it is very simple to do it is a matter of simple substitution, notice that these two terms cancel, this is plus or minus $i k$ square and this is k square.

So, now you are left with only these three terms in this bracket, and these three terms add up to go to 0, what does it tell us about the ratio of F double prime to F . Because, you can divide each of these three terms by the function F , so you got F double prime by F in the first, you have got F prime over F in the second, other than this constant plus or minus twice $i k$. And then you have got U which I have moved to the right hand side.

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~~$\frac{F_l''(k, r)}{F_l(k, r)} \pm 2ik \frac{F_l'(k, r)}{F_l(k, r)} = U_l''(r)$~~

Present interest \rightarrow
 $\rightarrow F_l(k, r)$: rather "slowly" varying function of r

$\Rightarrow \frac{F_l'(k, r)}{F_l(k, r)} \approx \frac{1}{\pm 2ik} U_l''(r)$

$F_l(k, r) = e^{\pm 2ik \int U_l''(r) dr}$

$U_l^{\text{effective}}(r) = U(r) + \frac{l(l+1)}{r^2}$

IF $V(r)$: Coulomb $U_l''(r) \rightarrow \frac{1}{r}$

$\int \frac{1}{r} dr = \ln r$

then $F_l(k, r)$: would **not** be independent of r

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Now, this is what we have got our interest let me remind you is in those cases for which F is a slowly varying function of r , what does it mean. If F was completely independent of r , f prime would be 0 and f by dr would be 0 right, so F prime is small it is not 0, but it is small. And F double prime will be smaller still right, so compared to F , F double prime is ignorable at least much more ignorable, than F prime.

So, if you look that first two terms, the left hand side the left hand side is a sum of two ratios, one is F prime over F , the second is F double prime over F . But, in our case F is a slowly varying function of r , which makes F prime weak and F double prime weaker still. So, the

first of these two terms is certainly ignorable compared to the second, do you recognize approximation here.

When you do that, you can throw off the first term, so for this case where F is rather slowly varying function of r , you throw off this term and you are left with this result. Now, you can actually integrate that because you have got $F' \text{ over } F$ and you know what it is integrals right.


So, you have got $F' \text{ over } F$ which is nearly equal to this plus or minus $1 \text{ over } 2$ while k comes here, and you have got effective potential which is a sum of the physical potential plus the centrifugal term. If you integrate this, you get F will be given by e to the power $1 \text{ over } \text{plus or minus } 2 \text{ i } k$ and the integral of this effective potential right, if you have an effective potential which you know is $U \text{ plus } l \text{ into } l \text{ plus } 1 \text{ over } r \text{ square}$.

Now, we recognize the constraints if the physical potential was a coulomb potential, then v would go as $1 \text{ over } r$ U which is proportional to v would also go as $1 \text{ over } r$. And as r turns to infinity $1 \text{ over } r \text{ plus } 1 \text{ over } r \text{ square}$ would go as $1 \text{ over } r$ because $1 \text{ over } r \text{ square}$ goes to 0 much faster than $1 \text{ over } r$ does. So, the effective potential will go as $1 \text{ over } r$ and the integral that you will need to determine over here, will be the integral of $1 \text{ over } r$ is that right.

So, if you have coulomb potential which is a common case, which is the case of the hydrogen atom actually right. If you had a coulomb potential, you would need the integral of $1 \text{ over } r$ and that would give you the logarithmic function, and you have e to this constant time logarithmic function, and what does it tell us for F , F would not be independent of r . We started by saying that our consideration will be valid for those cases, for which the potential is weak.

And then F must become only weakly dependent on r and it cannot be dependent on r , but if the potential that we are dealing with is actually coulomb potential. We find that F would not be independent of r , which means that this method is not going to work for the coulomb potential it does not. But, it does work for all potentials which go to 0 as r turns to infinity, faster than the coulomb potential, so that is the condition which is emerging from this analysis is this is the point I wanted to discuss. When I said that we are dealing with potentials which fall, whose physical influence falls off in the asymptotic region.

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....for potentials that
fall faster than the *Coulomb* potential,
i.e. faster than $\frac{1}{r}$ as $r \rightarrow \infty$
Coulomb case:
- different techniques are used.

See:
Landau & Lifshitz, Non-Relativistic Quantum Mechanics

Renu Mathai (M.Sc. 1987, IIT-Madras)
"The continuum eigenfunctions of the Coulomb potential"


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But, at what rate it must fall is given by this that the potential must fall faster than the coulomb potential, that the potential if it falls faster than $1/r$ as r tends to infinity. Then our method will be applicable for those potentials, which go as $1/r$ specifically the coulomb potential, somewhat different techniques have to be used, and some of our analysis is not applicable to it directly. It has to be modified one has to introduce what is called as coulomb phase shift, that requires different techniques.

And we would not have the time to discuss that, but you know this is nicely discussed most books on quantum mechanics, like Schiff's quantum mechanics, ((Refer Time: 15:25)) Schiff's are good sources, one of our master's students Renu Mathai had a very good report on the continuum functions of the coulomb potential. So, that copy should also be available in our lab, you can go through it and wish that the coulomb problem is discussed in great details.

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$$\text{When } \lim_{r \rightarrow \infty} |U(r)| = \frac{M}{r^{1+\varepsilon}}; \quad M: \text{constant and } \varepsilon > 0$$

$$y_l(k, r) = F_l(k, r) e^{\pm ikr} = B_l^{(1)}(k) e^{ikr} + B_l^{(2)}(k) e^{-ikr}$$

$$y_l(k, r) \xrightarrow{r \rightarrow \infty} c_1 \cos\left(kr - \frac{l\pi}{2}\right) + c_2 \sin\left(kr - \frac{l\pi}{2}\right)$$

$$y_l(k, r) \xrightarrow{r \rightarrow \infty} A_l(k) \sin\left(kr - \frac{l\pi}{2} + \delta_l(k)\right)$$

$$R_{el}(r) \xrightarrow{r \rightarrow \infty} \frac{y_{el}(r)}{r} \xrightarrow{r \rightarrow \infty} A_l(k) \frac{\sin\left(kr - \frac{l\pi}{2} + \delta_l(k)\right)}{r}$$

$$R_{el}(r) \xrightarrow{r \rightarrow \infty} A_l(k) \frac{e^{i\left(kr - \frac{l\pi}{2} + \delta_l(k)\right)} - e^{-i\left(kr - \frac{l\pi}{2} + \delta_l(k)\right)}}{2ir}$$

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But, we will restrict our discussion to those cases, those potentials which do go to 0 as r turns to infinity. But, at a rate which is faster than the coulomb potential, which is faster than 1 over r , so it is 1 over r , r to the power of 1 plus epsilon, epsilon could be no matter what; however, small, but it must be greater than 0 , if it is 0 this method it is not going to work. It could be small as long as it is small it will work, and in this case since F is nearly constant.

You can write the solution as a super position of e to $i k r$ and e to the minus $i k r$, this is the super position of spherical in going waves and spherical out going waves, you can do that. But, instead of writing this as a super position of spherical in going and outgoing waves, you can also write it as super position of sin and cosine functions, it does not matter because a function you can represent as a super position of linearly independent pair of function, and as long as the basis is complete you can use any basis.

So, you can use either spherically in going or outgoing waves, you can use the basal function at the Neumann functions or you can use the Henkel functions of the first kind and the second kind. So, they are alternative basis pairs that you can use, and here I have written this instead of the exponential functions, as a super position of cosine and sin functions. And once you have it, you can easily write it as sin of $k r$ minus $l \pi$ by 2 and add a phase shift here, because $\sin a$ plus b is $\sin a \cos b$ plus $\cos a \sin b$ and you get the previous form directly right.

So, instead of the constant c_1 and c_2 you have two other constants, which are a and δ , and you can get 1 as the tan inverse of the ratio of the other two terms, so it is a straight

forward thing to do. And what you discover is that your radial function, which is y divided by r is simply this sinusoidal function, which is the same thing as you get for a free particle with an additional phase shift and you write this sinusoidal function, again in terms of spherical outgoing waves, and spherical incoming waves.

And this is the form that we have used in our analysis in our previous class, so the phase shift does not [FL] come out of the blue, it is directly the consequence of the scattering potential. Nevertheless, there are certain conditions that the potential must satisfy, and in particular this method does not work in the case of coulomb potential, somewhat different techniques are to be used. But, for most of the potentials and most of the physical potentials that you work with r not exactly $1/r$ over potentials because there are other electrons and screenings and so on. So, in other case is you find that this is a fairly good approximation, and the radial function is then given by in terms of the spherical ingoing and outgoing waves.

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The slide contains two main equations and a note. The top equation is labeled "Phenomenological solution to the scattering problem" and shows the asymptotic form of the wave function $\psi_{k_i}^+(\vec{r}; r \rightarrow \infty) \xrightarrow{r \rightarrow \infty} A(k) \sum_{l=0}^{\infty} i^l (2l+1) \frac{e^{i(kr - \frac{l\pi}{2})} - e^{-i(kr - \frac{l\pi}{2})}}{2ikr} P_l(\cos\theta) + \frac{f(\hat{\Omega})}{r} e^{ikr}$. The bottom equation is labeled "Solution to the Schrodinger eq. $H\psi = E\psi$ " and shows the full wave function $\psi_{k_i}^+(\vec{r}) \xrightarrow{r \rightarrow \infty} \sum_{l=0}^{\infty} \sum_{m=-l}^l c_{lm}(k) A_l(k) \frac{e^{i(kr - \frac{l\pi}{2} + \delta_l(k))} - e^{-i(kr - \frac{l\pi}{2} + \delta_l(k))}}{2ir} Y_{lm}(\hat{e}_r)$. A red arrow points from the coefficients $c_{lm}(k)$ in the bottom equation to a yellow box that says "coefficients of e^{+ikr} must be equal". To the right of this box, the text "Use:" is followed by the equation $c_{lm}(k) = \frac{A(k)}{kA_l(k)} i^l \sqrt{4\pi(2l+1)} e^{+i\delta_l(k)} \delta_{m0}$. The NPTEL logo is in the bottom left, and "PCD STAP Unit 6 Atomic Probes CBS" and "57" are in the bottom right.

This is the form that we used to write the total wave function, and this pretty much completes the analysis that we completed in our previous class. I will go through some of the essential steps, just to reinforce the point that you have to the total wave function, which was written in terms of the spherical harmonics, and the basal functions with appropriate boundary conditions. And here there is a space shift delta coming due to the potential.

And then these C_{lm} these were the unknown coefficients, but then in these true forms this is the phenomenological expression, this is the total solution to the S_i equal to the e_{psi}

Schrodinger equation, these two solutions must be equal. And they must guarantee that the coefficients of the outgoing waves are equal, this coefficient involves c_{lm} , but this we have already used earlier. We obtained this c_{lm} explicitly in our previous class.

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The slide displays the following mathematical expressions:

$$\psi_{\vec{k}_i}^+(\vec{r}; r \rightarrow \infty) \xrightarrow{r \rightarrow \infty} A(k) \left[\sum_{l=0}^{\infty} i^l (2l+1) \frac{e^{i(kr - \frac{l\pi}{2})} - e^{-i(kr - \frac{l\pi}{2})}}{2ikr} P_l(\cos\theta) + \frac{f(\hat{\Omega})}{r} e^{ikr} \right]$$

$$\psi_{\vec{k}_i}^+(\vec{r}) \xrightarrow{r \rightarrow \infty} \sum_{l=0}^{\infty} c_{l,m=0}(k) A_l(k) \frac{e^{i(kr - \frac{l\pi}{2} + \delta_l(k))} - e^{-i(kr - \frac{l\pi}{2} + \delta_l(k))}}{2ir} Y_{l,m=0}(\hat{e}_r)$$

coefficients of e^{+ikr} must be equal

$$\sum_{l=0}^{\infty} \frac{A(k)}{k A_l(k)} i^l \sqrt{4\pi(2l+1)} e^{+i\delta_l(k)} A_l(k) \frac{e^{-i\frac{l\pi}{2}} e^{i\delta_l(k)}}{2ir} Y_{l,m=0}(\hat{e}_r)$$

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So, now you can set these coefficients equal, so you get the coefficient of the outgoing wave e^{+ikr} to the $i k r$ over here, you will get the $A(k)$ you will get the sum over l $2l+1$ plus 1, you have this e^{+ikr} to minus $i l \pi$ by 2, which is which is coming here you have got the 1 over $2 i k r$ which is here. You have got the legendary polynomial, and then from this term you have got the scattering amplitude and 1 over r .

So, this is the term which multiplies the spherically outgoing wave, in this form and the lower form you have got and exactly you do the same thing extract the coefficient of e^{+ikr} . In which you also have the c_{lm} , so you plug in the c_{lm} from the result that you have obtained from the previous class, and now all you have to do is to equate this with this, those are the two coefficients of the spherical outgoing waves.

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equating the coefficients of e^{+ikr} :

$$A(k) \left[\sum_{l=0}^{\infty} (2l+1) \frac{1}{2ikr} P_l(\cos\theta) + \frac{f(\hat{\Omega})}{r} \right] =$$

$$= \sum_{l=0}^{\infty} \frac{A(k)}{k A_l(k)} i^l \sqrt{4\pi(2l+1)} e^{+i\delta_l(k)} A_l(k) \frac{e^{-i\frac{\pi}{2}} e^{i\delta_l(k)}}{2ir} Y_{l,m=0}(\hat{e}_r)$$

$$\left[\sum_{l=0}^{\infty} (2l+1) \frac{1}{2ik} P_l(\cos\theta) + f(\hat{\Omega}) \right] =$$

Canceling common terms on lhs & rhs $= \sum_{l=0}^{\infty} (2l+1) e^{+2i\delta_l(k)} \frac{1}{2ik} P_l(\cos\theta)$

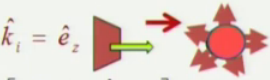
$$f(\hat{\Omega}) = \sum_{l=0}^{\infty} \left[(2l+1) \frac{e^{+2i\delta_l(k)} - 1}{2ik} P_l(\cos\theta) \right]$$


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So, once you equate them and then you cancel common terms simplify, and essentially you get the Faxen Holtzmark's scattering amplitude. Because, you have this scattering amplitude over here, you move this term to the right and you get this e to the $2i\delta_l(k)$ minus 1 over $2ik$ which is the scattering amplitude.

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

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

Faxen-Holtzmark's formalism

Contributions of the partial waves to the scattering amplitude.



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So, it is a very simple analysis and this is sometimes referred to as partial wave method because there are, so many partial waves with different l quantum number, which contribute to the scattering amplitude. There are infinite of those because l goes from 0 to infinity, the

linear momentum is a good number for free particles, but angle of momentum is not. And therefore, you need the superposition of the entire basis which includes l going from 0 to infinity, and it would be a very burdensome competition if you had to do all of these infinite partial waves.

But, you do not really have to because as l increases the radial function of the continuum, the radial part of the continuum function will go as r to the power of l . And it will not be able to penetrate into the core into the scattering region, so only a few partial waves have to be considered. And we have done calculations in which only about 8 to 10 partial waves l equal to 0 up to l equal to 8 or 10 are sufficient. Sometimes you need more than that you can take 10, 20, 50, 100 people and even do a 1000, but certainly not infinite. And even 1000 is a tangible number, it is not something which is not manageable, and the centrifugal barrier is the main reason that you can truncate this partial wave expansion to certain limit.

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To proceed, we first show the equivalence of two forms of the incident plane wave

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

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

Then, we shall write the total wave function in a similar form, like (2), and then discuss 'normalization' and 'boundary condition' for collisions / photoionization

$$\psi_i(\vec{r}) \xrightarrow{r \rightarrow \infty} A \left[e^{i\vec{z}} + \frac{f(\hat{\Omega})}{r} e^{ikr} \right]$$

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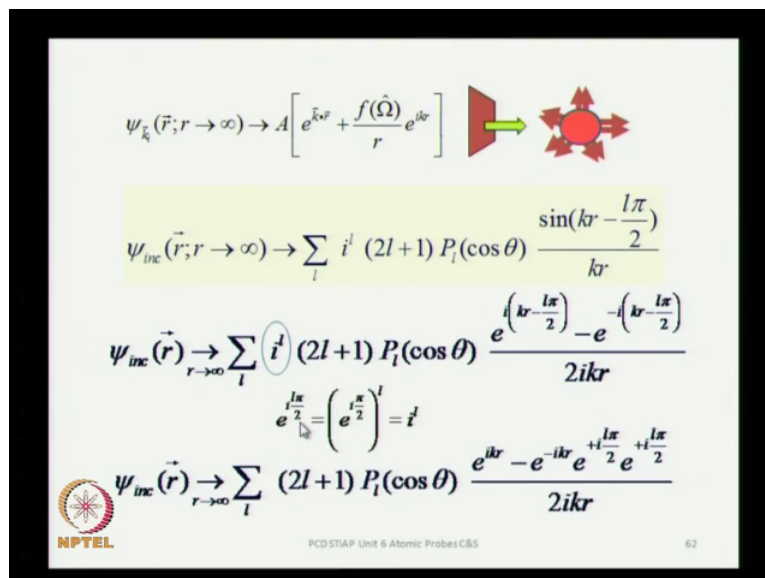
Now, we are going to get the boundary conditions and we will see how these boundary conditions are recognized, we have already been discussing these boundary conditions. We already use these boundary conditions, but we will discuss them further to recognize a particular element in the boundary condition, which is of importance and to be able to do that, we first write the incident plain wave which is this in equivalent form over here.

This is completely equivalent form, but I will demonstrate very quickly how this is these two forms are equivalent. And once we do that, we will write the total wave function also in a

form which is similar to this second form, and then we shall proceed to discuss the boundary conditions, these boundary conditions are different for collisions. And for photo ionization, our eventual goal in this discussion is to relate the boundary conditions for photo ionization and collisions.

And we have already seen in some of the diagrams that I have discussed earlier that they both have the same final state, but the initial states are different and there is a certain time reversal symmetry, which is involved which connects the two. So, that is our goal for this discussion we will get to that, and to be able to get to that we first want to write the total wave function also in a form, which is similar to this second form. So, let us write that, this is hung up a little bit alright.

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

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

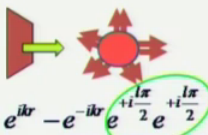
$$\psi_{inc}(\vec{r}) \rightarrow \sum_l i^l (2l+1) P_l(\cos \theta) \frac{e^{i(kr - \frac{l\pi}{2})} - e^{-i(kr - \frac{l\pi}{2})}}{2ikr}$$

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

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

So, this is your incident plane wave this sinusoidal function you write as $e^{i\vec{k} \cdot \vec{r}}$ to the minus $e^{i\theta}$ to the minus $i\theta$ divided by $2i$, and this i to the l you write as $e^{i\frac{l\pi}{2}}$ by 2 . So, you can multiply both of these terms by $e^{i\frac{l\pi}{2}}$ that will cancel this $e^{i\frac{l\pi}{2}}$, and here you will get $e^{i\frac{l\pi}{2}}$ into $e^{i\frac{l\pi}{2}}$, so you will get $e^{i\frac{l\pi}{2}}$ in the second term right.

(Refer Slide Time: 25:42)



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

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

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

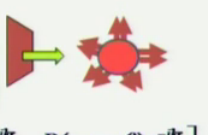
$$\psi_{inc} \xrightarrow{r \rightarrow \infty} \frac{1}{2ikr} \sum_l (2l+1) \left[P_l(\cos \theta) e^{ikr} - P_l(\cos \theta) (-1)^l e^{-ikr} \right]$$

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

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So, that is what you have got minus 1 to the l because e to the i pi is minus 1 right, so now, you have got the incident wave which is the plane wave which is written in the form of legendary polynomials. And you have got this spherical outgoing wave and spherical ingoing wave, which is multiplied by minus 1 to the l and this minus 1 to the l you take this p l cos theta, and multiply both of these terms by p l cos theta you have got p l cos theta into minus 1 to the l, what is p l of minus cos theta right. So, that is what it is you have got the legendary polynomial for minus cos theta over here, so this is your incident wave.

(Refer Slide Time: 26:36)



$$\psi_{Tot} = \psi_{inc} + \psi_{scat}$$

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

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

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

$C_l = e^{i\delta_l(k)}$ How should the normalization $\textcircled{C_l}$ be chosen so that we get correct $\psi_{scattered}$?

$$\psi_{scat} = \frac{e^{ikr}}{r} \left\{ \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \left[e^{2i\delta_l(k)} - 1 \right] P_l(\cos \theta) \right\} f(\hat{\Omega})$$

Normalization: outgoing wave boundary conditions

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So, you have got your $P l \cos \theta$ into the $i k r$ and $P l$ of $\cos \theta$ into e to the $\cos \theta$. And now let us write the total wave function, in exactly the same form this is also written as $P l \cos \theta$ into $i k r$, but now we know that the total wave function must have the scattering phase shift δl , the coefficient of e to the $\cos \theta$ is again is $P l \cos \theta$ is exactly as the same we know, except that there is an additional phase shift.

So, that goes over here right, but then you do not know what is $c l$, this is the unknown coefficient in the total wave function. The question is how will you determine the $c l$, what is the boundary condition which gives you the $c l$, this is I know this is what you have to find out. Now, we do know that the total wave function is the sum of incident wave and the scattered wave right. So, you have got the incident wave, you also have the total wave.

So, if you subtract the total wave from the incident wave, you must get the scattered wave, and that condition will give you what the $c l$ must be. And now you know what the scattered wave is, scattered wave is known is it not this is the scattered wave e to the $i k r$ over r multiplied by the scattering amplitude, we have just determined that right. So, now tell me what the $c l$ should be because all you have to do is to subtract this incident wave from the total wave to give you the scattered wave, you have got all the pieces now tell me what should be value of $c l$ got it.

You should just get it by observation, if you were listening what should be $c l$, what value of $c l$ will give you the scattered wave. It cannot take time come on if you just take a look at one of the terms you will get it do not even have to see, you want to remove this part what is it, you got $p l \cos \theta e$ to the $i k r$ come on I think you are not even trying, it is very easy no it is too simple.

Student: ((Refer time: 29:46))

If you look at any one of these terms, there are two terms how do you subtract this term from this term, to get this. This one has nothing in the e to the $\cos \theta$ right, all you need is put $C l$ equal to e to the $i \delta l$ that is all you need to do. If you put C equal e to the $i \delta l$ that is it, do you see it you are not even trying I am afraid it is taken care of you got e to the $\cos \theta$ $i \delta l$ here. So, that is what gives you the C to the $2 i \delta l$ here right. So, this is the beautiful result that the choice of the coefficient, and this is an extremely important choice.

Because, this is what determines that the process you are talking about is a collision phenomenon, we know that the answer is a collision scattering amplitude right, which is what gives you the Faxén, Holtzmark's scattering amplitude right. And you get it by choosing C_l to be $e^{i\delta_l}$ for you know until we recognize it to be this $e^{i\delta_l}$, it is just the multiplicative factor in the superposition right. It is an arbitrary multiplicative factor, but it no longer remains arbitrary what is it that pins it down.

It is a boundary condition that the solutions will give you the scattering, the solution to the scattering problems which is the sum of this incident plane wave plus a spherical outgoing wave, scale by $1/r$ and an angle dependent scattering amplitude that is the boundary condition. And this choice is completely equivalent to C being $e^{i\delta}$, now notice this will also the value of C will also affect the normalization.

So, when you make this choice you often say that you have normalized the solution, according to the outgoing boundary wave function. Because, that is what you have in your scattered part, in the scattered part you have got a spherical outgoing wave that is the only thing you have got in the scattered part of the function.

There is no ingoing component in the scattered wave, which is why this is called the normalization according to the outgoing wave boundary conditions. So, this is normalization according to the outgoing wave boundary condition, and you have got the scattering phase shift, which we know is coming from the potential itself.

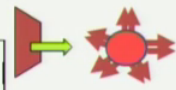
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$$\psi_{Tot} = \psi_{inc} + \psi_{scat}$$

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

ψ_{Tot}
 $r \rightarrow \infty$

→




choice: $c_l = e^{i\delta_l(k)}$

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

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

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

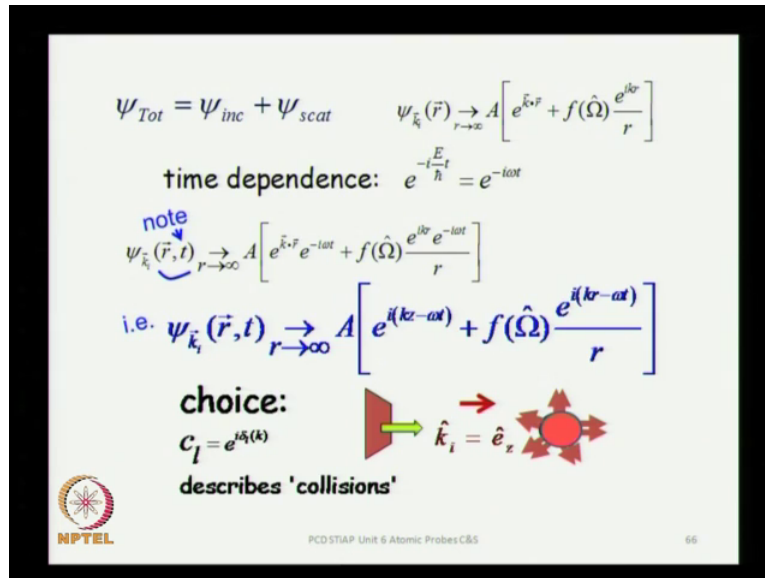


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Now, let us look at the solution further this is our total wave function, and we will put in the value C equal to the i delta l in this, and with this you have got this total wave function which is given as e to the i delta l will give you this particular solution.

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

time dependence: $e^{-i\frac{E}{\hbar}t} = e^{-i\omega t}$

note

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

i.e. $\psi_{\vec{k}_i}(\vec{r}, t) \xrightarrow{r \rightarrow \infty} A \left[e^{i(kz - \omega t)} + f(\hat{\Omega}) \frac{e^{i(kr - \omega t)}}{r} \right]$

choice:

$c_l = e^{i\delta_l(k)}$

describes 'collisions'

Diagram: A red arrow points from a red rectangular barrier to a red dot. From the red dot, several red arrows radiate outwards, representing scattering. The incident wave vector is labeled $\hat{k}_i = \hat{e}_z$.

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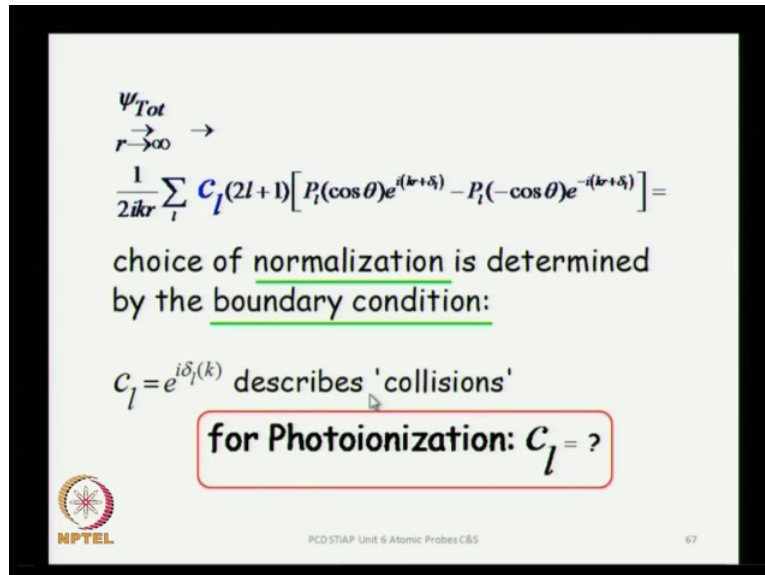
And let us try this together with the time dependent term because that is more important to see. Because, the net wave function must be multiplied by this e to the minus i omega t that is the thing that tells you whether the wave is a travelling wave, where it travels from left to the right or right to the left, from the centre to farther away or in the other direction. So, when you put this e to the i omega t you get k z minus omega t from here and k r minus omega t. So, you recognize this as a plain wave, and this as a spherical outgoing wave.

So, this is the picture that we have been using everywhere, and this picture now really makes sense. Because, it shows how a surface of constant phase propagates, this travel is of importance this is what tells you, what nature of the solution without the time dependence actually it does not mean anything e to the i k z is not necessarily a function, which is moving along the plus z axis. What determines is what is d z by d t is d z by d t positive or is it negative, if it is negative it would actually be a wave that is going in the negative direction.

So, likewise e the i k r by itself does not determine that it is a spherical outgoing wave, the argument with reference to time is k r minus omega t. So, that the surface of constant phase will be given by k r minus omega t being a constant, and that will require d r by d t to be given by a positive number. And since d r by d t is positive, you have got the radius of the

surface of the constant space which increases that is what makes it a spherical outgoing wave. So, now our solution is complete inclusive of the time dependent term, and what gives us this corrective form is the choice C equal to $e^{i\delta}$, and this is of tremendous importance in our discussion of photo ionization.

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

choice of normalization is determined by the boundary condition:

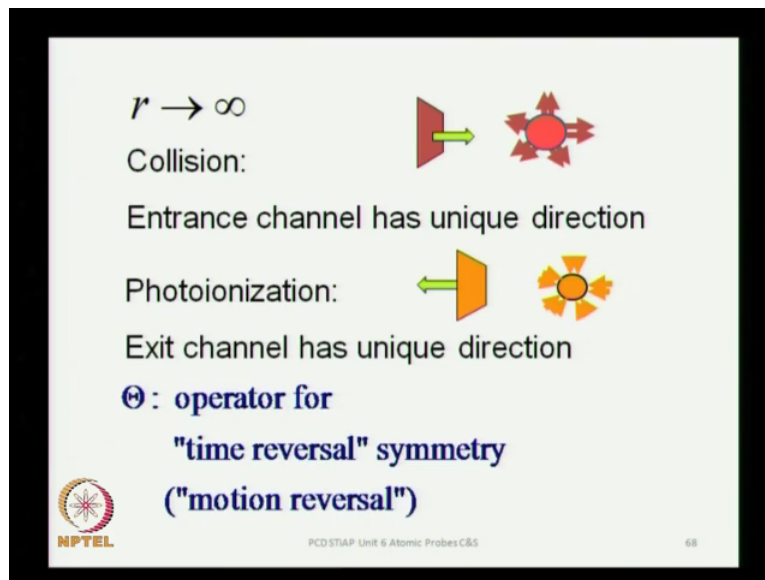
$C_l = e^{i\delta_l(k)}$ describes 'collisions'

for Photoionization: $C_l = ?$


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So, this is what is called as normalization as per outgoing wave boundary condition, this scattering phase shift gives you a coefficient, which describes the collision phenomenon. And the question that we are going to ask now is, what boundary condition will describe the photo ionization, we know that C_l equal to $e^{i\delta_l}$ will describe the collision how should c be chosen. So, that we describe the photo ionization that is the next question we want to ask, we know that there is a certain similarity, we know that both of these operations have got the same final state, but different initial states even the initial ingredients are different.

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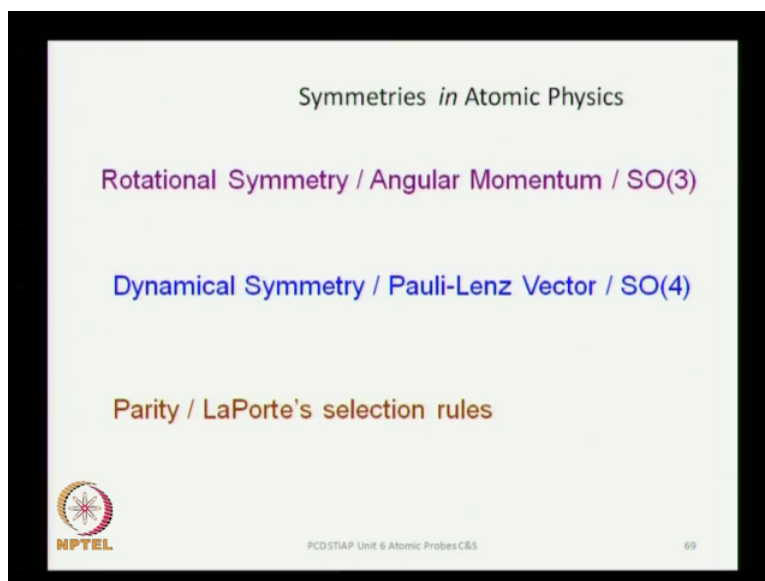


So, now let us begin to look at the photo ionization event in which as I discussed earlier, you have got a photoelectron in the final state. So, you have got a certain central region an atomic system of quantum atomic system, which has absorbed electromagnetic radiation, an electron has been knocked out through the photoelectric effect it goes into the continuum. And you sense it in a certain detector, and this direction in which the photoelectron has escaped is unique.

So, the exit channel has got a unique direction in the collision it was just the opposite, in the collision you had a scattering centre, you had the electron gun at one place and this electron gun fired the electrons toward the target. So, this entrance channel was unique, so in photo ionization it is the exit channel which has got the unique direction, and if you see that if you were to take a picture of this process.

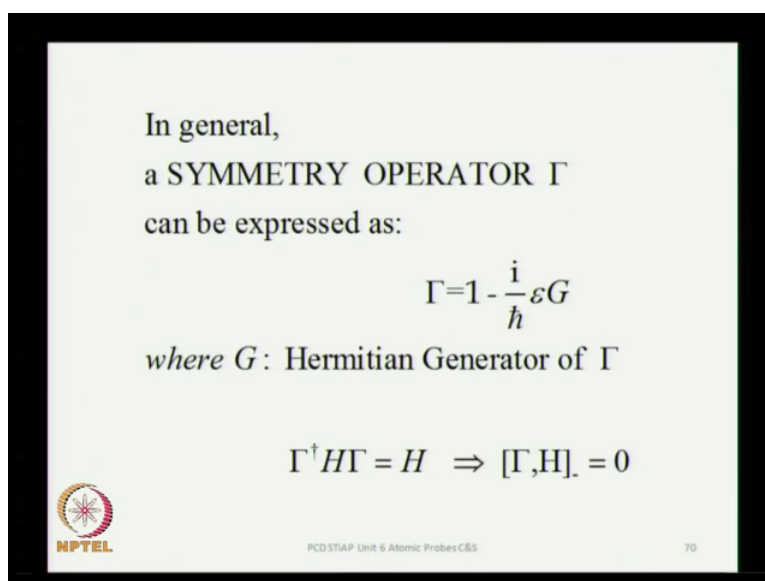
And imagine this being recorded on a film this process would be somewhat similar to a film, which is being run backward in time. So, I suggest it to you that it has something to do with time reversal symmetry, and we now need to discuss what is meant by time reversal symmetry in quantum mechanics, and how does it connect the solutions of photo ionization to collisions.

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So, there are symmetry plays an extremely important role in all physical phenomena, and of course, in atomic processes as well. We first dealt with the rotational symmetry, the generator for rotations are the angle for momentum operators, they gave us the SO 3 algebra right. Then, we also discussed the anatomical symmetry of the hydrogen atom coming from the SO 4 symmetry right. Then there is parity, and parity is also important in atomic processes you have seen the dipole selection rules as an application of wignereckart theorem, you know that dipole transitions take place only when parity changes. So, there are these parity selection rules which are of importance, but then there are many other symmetries.

(Refer Slide Time: 39:45)



And typically a symmetry is an operator which you can write as $1 - \frac{i}{\hbar} G \epsilon$, and when G is a hermitian generator of the symmetry ϵ that is a typical symmetry of an operation. Because, it gives you a gamma an operator which commutes to the Hamiltonian, so the Hamiltonian remains a variant under that operation that is the idea of a symmetry.

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Dynamical symmetry Geometrical/spatial

$SO(4) \rightarrow$ Unit 1 Translation: spatial displacement

$\tau(\vec{dx})|\vec{x}\rangle = |\vec{x} + \vec{dx}\rangle;$ $\tau(\vec{dx}) = 1 - \frac{i}{\hbar} \vec{p} \cdot \vec{dx}$

Generator of translational displacements - Symmetry Operator

Rotation: angular displacement $U_R(\delta\vec{\phi}) = 1 - \frac{i}{\hbar} \delta\vec{\phi} \cdot \vec{J}$

Translations/Rotations **other symmetries**

UNITARY TRANSFORMATIONS Π : *parity*

Continuous Θ : *time – reversal*

Discrete

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So, now the dynamical symmetry we have discussed at length in unit 1, so far as the geometrical symmetries are concerned, you have the translational symmetries generated by the linear momentum, which is conserved in a translational homogenous phase. You also have the angle momentum, which is the generator of rotations and these are as you can see from both of these operators, we generate the corresponding you know translations or rotations these are unitary transformations.

They are also continuous transformation, in homogenous phase you can move infinitesimally, this is generator δx is the generator of infinitesimal translation $\delta \phi$ is a generator of infinitesimal rotations. So, these are continuous variables, but then there are discrete symmetries, like parity and time reversal these are discrete symmetries. Parity you go from one space into the other which is the mirror space right, and you do, so one shot.

Time reversal is again a discrete symmetry, because from a certain time t you go to minus t there is nothing in between. It is not like a number 0.5 on a real number axis which you reduce to 0.4 then to 0.3 then to 0.2, 0.1, 0 and then minus 0.1 and so on, you do not do, so

continuously, you do this with angles, you do these with translation, but you do not do this with time reversal nor with parity. So, these are discrete symmetries just like charge conjugation, you go from the electron to positron there is nothing in between.

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The slide is titled "Discrete symmetry" and is divided into two main sections. The left section, titled "Discrete symmetry", features a small image of a green, glowing, elongated object with the text " Π : parity" overlaid. Below this, it lists "Other discrete symmetries" with bullet points for "Charge conjugation" and "Time Reversal". The right section, titled " Π : parity", discusses "electroweak unification - Glashow-Weinberg-Salam" and cites "D Budker, D F Kimball and D P DeMille, Atomic Physics: An exploration through problems and solutions, Oxford Press, 2004." Below this, it states "present interest:" and lists " Θ : time reversal". At the bottom, there are two diagrams: the left one shows a red arrow pointing right and a red star-like shape, and the right one shows a green arrow pointing right and a yellow star-like shape. The NPTEL logo is in the bottom left corner, and the text "PCD STAP Unit 6 Atomic Probes CBS" and "72" are in the bottom right corner.

So, this is the discrete symmetry and you know that the parity is violated in the electroweak interaction, the weak interaction beta d k is violated right, and since electroweak force is the same force. Atomic processes being governed mostly by electromagnetic phenomena, but then electromagnetic interaction is not different from the weak interaction, you would expect the parity to be violated in the atomic processes as well. Because, it is the same interaction right and yes there is a quest for parity violating phenomena, many have been observed in atomic physics.

And we will not have time to discuss those aspects in this part of the course our focus here is on collision and photo ionization. Then there is this charge conjugation as well as the time reversal, our interest is related to these two phenomena and how the time reversal symmetry connects solutions of collisions to the solutions of photo ionization that is our focus in the present discussion.

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CP violation was discovered in 1964, but it has been observed only in the decays of the neutral K mesons.

CP violation → matter / anti-matter asymmetry

CPT Symmetry

Dipole moment of a particle must be zero unless

T symmetry is broken No eEDM has yet been found.

eEDM search in heavy polar molecules (YbF)
cheaper than LHC!

ENHANCEMENT FACTOR!

Symmetry in Electron-Atom Collisions and Photoionization Process
Pranava C. Deshmukh, Dilip Angom, and Alak Banik
https://www.physics.illinois.edu/~habibulaziz/homepage/OST_SERC_School_Publications/PCD-102-SEACP.pdf

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But, then remember the CP violation has been observed, and if CP is violated then time reversal symmetry is also ought to be violated, then you can look for that in atomic physics also. And if it is violated in atomic physics, where will you find it, you will find that you will have these electrons to have a certain dipole moment, so you can look for certain dipole moment.

And if you find it would be the evidence of the breakdown of the t symmetry, and that would be wonderful this experiment will be much cheaper than what it is at the large hadron collider. You can do it in the lab and people are looking for this, you they do not only for the atomic systems, but actually for molecules because there is a certain enhancing factor which enables which gives you some comfort because the probability of detection goes up very much because of that.

CP violation is of importance some of you keep wondering where is all the antimatter, part of the reason you do not find as much of the antimatter as you find matter is because of CP violation, but that is again involved question which that does not fall into the scope of our discussion.

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Classical equations of motion:
Symmetric with respect to $t \rightarrow -t$

Let for particle I: $\vec{r}_I(t=0)$ and $\vec{p}_I(t=0)$

Let for an indistinguishable particle II:

$\vec{r}_{II}(t=0) = \vec{r}_I(t=0)$
and $\vec{p}_{II}(t=0) = -\vec{p}_I(t=0)$

If $\vec{r}_{II}(t) = \vec{r}_I(-t)$ then, motion
**and $\vec{p}_{II}(t) = -\vec{p}_I(-t)$ has Time Reversal
symmetry**



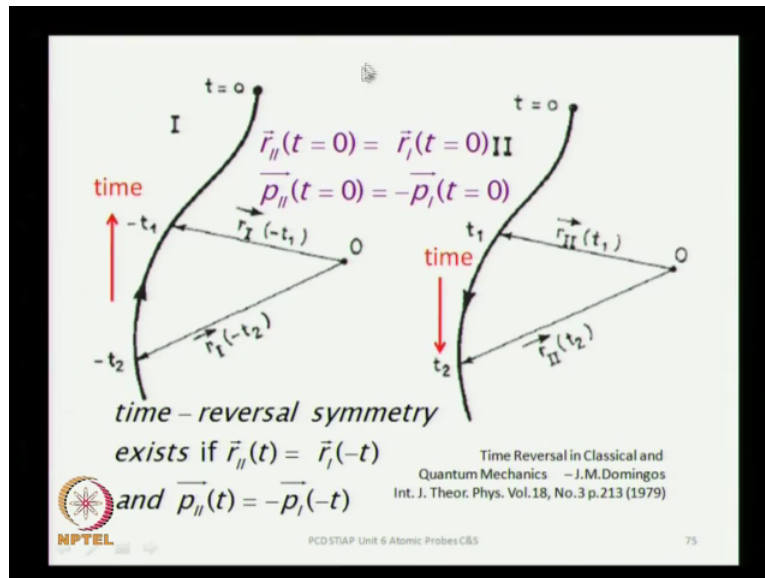
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We will nevertheless need to understand what exactly is meant by time reversal symmetry. And it is not the same as classical mechanics, so let us first understand what time reversal symmetry means in classical mechanics. So, classical equations of motion are symmetric with respect to t going to minus t , and what this means is that if you have particle one, which is at position vector \vec{r}_1 and momentum vector \vec{p}_1 at t equal to 0.

And if there is an identical particle, this is particle two whose position at t equal to 0 is the same as the position of particle 1 equal to 0. But, this momentum is opposite it is linear momentum is opposite, then if these relations hold that at a later time the particle two will have the same position as particle one had at a previous as much time. So, this is t going to minus t , so at a previous as much time if the second particle has the same position, as the first particle had at as much previous time. And the momentum is the negative of what the first particle had, at that much previous time, which is minus of \vec{p}_1 minus 2. Then you say that motion has time reversal symmetry, this is the meaning of time reversal symmetry in classical mechanics.

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And in classical mechanics it is very easy to deal with because this is the picture which shows you, how the definition which I just provided this is the position of these two particles, particle one and particle two at equal to 0, and this momentum of these two particles at equal to 0, except that the momentum of the second particle is opposite to that of the momentum of the first particle. And this is the criterion for time reversal symmetry, this diagram is from a very nice article by Domingo's I will strongly recommend this article, in which he discusses time reversal in classical mechanics and in quantum mechanics.

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Classical equations of motion:
Symmetric with respect to $t \rightarrow -t$

$\vec{r}(t)$ and $\vec{r}(-t)$: both are solutions of the 2nd order Newton/Lagrange equations.

$\dot{q} = \frac{\partial H}{\partial p}$ and $\dot{p} = -\frac{\partial H}{\partial q}$ First order equations,
but note asymmetry in sign that is involved in the above two equations

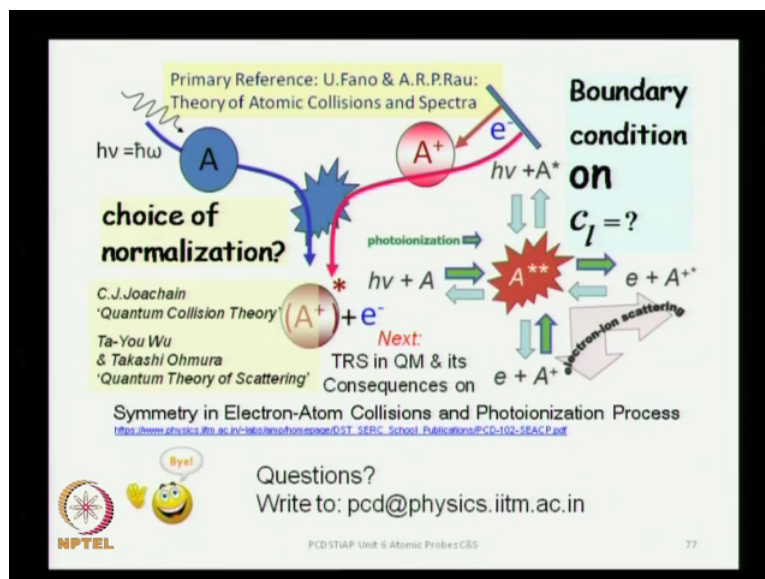
TRS? Q.M. $\rightarrow i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} = \left[\frac{(-i\hbar \vec{\nabla})^2}{2m} + V(\vec{r}) \right] \psi(\vec{r}, t)$

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So, classical equations of motion are symmetric with respect to t going to $-t$ because both $r(t)$ and $r(-t)$ are solutions to Newton's laws or Newton's equation of motions and also to the Lagrange's, both are second order differential equations right. So, d^2 by dt^2 as t goes to $-t$ remains the same, same thing happens with the Lagrange's equations, Hamilton's equations are first order equations. But, then there is a minus sign here, so that takes the care of it, so all classical equations whether Newton, Lagrange or Hamilton of course, they are equivalent to each other.

So, no wonder, but it is obvious that they are symmetric under time reversal t going to $-t$, the question is what does time reversal symmetry mean in quantum mechanics where the evolution of the system is described not by Newton's equation or Lagrange's or Hamilton's equations. But, by the Schrodinger's equation, and this is the rate equation $\frac{d\psi}{dt}$ tells you how the system evolves with time. So, what is time reversal symmetry in quantum mechanics, and this is what we will discuss in our next class, and then connect the collisions and photo ionization.

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So, that will be our point of discussion for the next class we do expect the solutions for photo ionization to be related to the solutions of the collisions experiment. Because, they have the same final state, you can see that from these two diagrams that we have discussed earlier. And this relationship is actually what connects the collision boundary conditions to the photo

ionization boundary conditions, then the connections will emerge from the time reversal symmetry in quantum mechanics.

So, with this I will conclude today's class essentially the question boils down to how do you choose the normalization C_l equal to the $e^{i\delta_l}$ is what gave us the correct boundary condition to describe the collision process. So, the question is how are we going to choose C_l to describe photo ionization, so that is the question we are going to answer there are a few references most of this discussion is from Fano and Rau it is a very nice book. And there are some other sources which I have suggested over here, if there are any questions I will be happy to take, otherwise we proceed from this point to the next class.