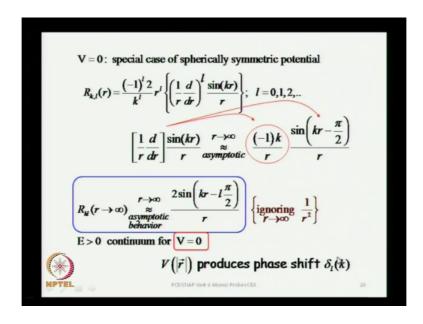
Select/Special Topics in Atomic Physics Prof. P. C. Deshmukh Department of Physics Indian Institute of Technology, Madras

Lecture - 27 Atomic Probe Collisions and Spectroscopy - Boundary Conditions

Greetings, we introduced Collisions and Spectroscopy as processes which are related, but we are yet to explode the detailed, relationship between these two processes. And it will take us a little while, before we actually get to the see the connections, so prior to that we need to lay down the foundations of collision, dynamics. And we started looking at that problem, by setting up collisions by spherically symmetric potentials.

And to solve the quantum mechanical problem, we thought that it will be a good idea following text, like Lyondell and Lifschitz, non relativistic quantum mechanics from which I have borrowed significant part of this material. What you do is first setup the problem, the quantum mechanical problem for V equal to 0, which is a special case of a spherically symmetric potential. Then solve it only for I equal to 0, only for the S wave function, S orbital's And then find out if you can have some sort of a recursion relation, so that from the solution for I equal to 0, if you can get solutions for higher values of I. And we discovered that such a recursion relation indeed exists.

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And you can get for this problem of V equal to 0 for the free particle, a solution which you can obtain from that of the solution for the S orbital, and all you need to do is to operate by this operator 1 over r d over d r, on this function sin k r over r which is a solution for l equal to 0. Now, you need to operate l times, and every time you operate by this operator, you get the same function which is a sinusoidal function divided by r. But, the argument of sinusoidal function is phase shifted, it is no longer k r as it was for l equal to 0, but it is phase shifted.

And it drops by a factor of phi by 2 every time you operate by 1 over r d d over d r, because the next time you operate on this function, once again you will get a term in 1 over r square. And that term in 1 over r square, you can ignore with respect to the term in 1 over r, every time you take the derivative you will get from the sine function, the derivative of the sine function will give you the cosine function; you will get a multiplicative factor of k. Because, the derivative of sine k r is cosine k r times k, so you will get multiplicative factor of k, but the cosine function is the same as the sine function except for the phase shift.

You get the sine function from the cosine function, simply by moving it along the independent degree of freedom, which is the angle through phi by 2. So, you will get a phase shift of phi by 2 and that is what gives you this net radial function, and because there is a factor of minus 1 over k minus 1 times k over r, this will get multiplied 1 times, it will get multiplied to itself 1 times. So, the r to the 1 factor will cancel ((Refer Time: 04:27)) this r to the 1, the k to the 1 will cancel this k to the 1 in the denominator, the minus 1 to the 1 will take care of this minus 1, which will be raised to 1.

And the net solution for the 1 th state, but for the case of V equal to 0, it will be given in terms of the solution for the 1 equal to 0, in which the argument of the sine function is phase shifted by 1 phi by 2. And this is the result, it is an approximate result, but good enough because the terms that are ignored are the terms in 1 over r square are weaker and therefore, this is a fairly acceptable solution; so this is the solution that we shall be using. Now, above in phase of course, is in having a real potential and what the potential does is that this argument k r minus 1 phi by 2 is further displaced by another phase shift.

So, the you will get a solution which will again be a sinusoidal function, but the argument of that function will be k r minus l phi by 2 plus a certain phase shift, which will depend on the l quantum number, the orbital angle of momentum quantum number, it will depend on the energy. So, it is written as delta l k, this is called as the scattering phase shift and you would

expect it to have intimate relationship with the whole scattering process. And all the physical information about the collision dynamics will be contained in the scattering phase shift, the reason is it is the quantity, it is the physical factor, which is affected by the potential.

The rest of the solution is due to a free particle, what the target does and that is precisely your object of interest, what the potential does is to cause this phase shift. So, a study of this phase shift will give you physical information about the target, which is the object of doing this collision experiments at all.

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

$$e^{i\vec{k}\cdot\vec{r}}=e^{ikr\cos\theta}=e^{i\rho\mu}$$

$$\text{with }\rho=kr\text{ and }\mu=\cos\theta$$

$$e^{i\vec{k}\cdot\vec{r}}=\sum_{l=0}^{\infty}\sum_{m=-l}^{+l}c_{l,m}Y_{l}^{m}(\hat{r})j_{l}(\rho)=\sum_{l=0}^{\infty}a_{l}P_{l}(\cos\theta)j_{l}(\rho)$$

$$e^{i\rho\mu}=\sum_{l=0}^{\infty}a_{l}P_{l}(\mu)j_{l}(\rho)$$

$$q_{l}=?$$
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So, this is your phenomenological solution, that you have got an incident plain wave and then the incident projectiles are scattered in various directions, the scattering probability will not be necessarily the same in all directions. So, there is an amplitude factor which is called as the scattering amplitude, so f of omega, omega is a direction vector it is an unit vector in a certain direction. So, it has got two parameters theta and phi, both the angular coordinates are contained in omega, the 1 over r takes care of the fact that there is no change in the flux after the scattering takes place.

So, that whatever flux is emitted in the certain solid angle that will be conserved, and that will get reduced as you go further away, because it is going to meet a solid angle which sort of envelopes the scattering region, a spherical envelope will have an area of 4 phi r square. So, since the area of the sphere goes as r square, the 1 over r which is sitting in this relationship over here, takes care of the conservation of the flux and then there is a spherical

outgoing wave as we discussed in our previous class. So, this is the phenomenological solution, this is a depiction of the physical process essentially.

So, what we will do is analyze these solutions, and it is important that you have the right attitude toward this class, because it will involve a good amount of mathematical relationships. But, the physical ideas are very simple, when you sit down to do it, it take some time one can make some careless mistakes, but if you follow the physical idea it is really very simple. And the only physical ideas which are of importance, there are very few and I will tell you what they are, the plain wave for example, you can represent it in a basis of spherical harmonics.

The net total solution to the problem, which is h psi equal to e psi that is your full description of the quantum mechanical problem, it has got solutions psi and these solutions can also be expressed in spherical harmonics. So, now you have got a very basic idea here that you got a phenomenological solution in front of you, which is e to the i k dot r plus f over r e to the i k r this is one solution. The solution is what you will get, the other solution you will get is by solving the Schrodinger equation, so you will get f psi equal to e psi.

And that solution you can also express in a basis of spherical harmonics, so now you have two alternate expressions for the solution, in the same basis sign. So, when you have a function which has got two expressions, at one linearly independent basis at, then the coefficients of the corresponding base functions must be equal that is all the rest to it. That is the only idea which is of important in all these mathematical, manipulation of the terms that we will be carrying out in today's class, the essential idea is only this.

So, do not worry about substituting the term one by one and figuring out how it is done, because all of these slides are uploaded on the course web page, so you will be able to go through that in details. So, concentrate only on this idea that all you have to do is to look for the coefficients of corresponding base functions, in two alternate expressions of a wave function in a linearly independent basis, it is a very elemental idea in quantum mechanics. Then there are a few other things and I will anticipate one result which I will be discussing in the next class, not in today's class, which is this effect of the potential which I have mentioned.

When you have a potential which is present, it will result in a sinusoidal solution once again, but in addition to the phase shift, which is k r minus l phi by 2, there will be an additional

phase shift. So, this result I will anticipate, I will discuss this result in further detailed in the next class as to how it is obtained. And in fact, it is realizable for certain kinds of potential, it is not for every spherical potential that you can do this. In fact, you cannot do it for 1 over r which is the coulomb potential, but this is the matter of detail which I will be discussing in the next class.

So, now let us look at this ((Refer Time: 12:16)) expansion of e to the i k dot r, which is the plain wave we know that mono energetic beam is represented by a plain wave. And this is the way which is moving from left to along the z axis, this is how the z axis has been set up in our pictorial representation of the collision process. And you can represent this expand it in spherical harmonics, so these are the spherical harmonics y l m theta pi or y l m theta pi is represented by this unit vector r, the radial part is given by the spherical Bessel functions.

And because of the symmetry, the symmetry about the z axis, you do not really have any five dependence and you have only the theta dependence, so you have only the Legendre polynomials coming in. So, this is the expansion of e to the i k dot r in Legendre polynomials, now the question is what are these coefficients a 1, j 1 of rho these are the spherical Bessel functions, these are the solutions to the radial part of the Schrodinger equation. And we know what is the radial part of the Schrodinger equation? We can solve it, we know the solutions are sinusoidal functions sine of k r minus 1 phi by 2 by r, those are the solutions for the radial part with appropriate phase shift due to the potential.

So, we already know the solution to the radial part, the angular part solutions also we know these are the spherical harmonics, once you solve the problem for any central field, you have got the spherical harmonics for I equal to 0, 1, 2, 3 everything. So, you have got the solutions with you, the only thing that you want to determine here is the coefficient a 1.

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

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

$$= \sum_{l=0}^{\infty} a_l \left[\frac{2}{2l+1} \delta_{l'l} \right] j_l(\rho)$$

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

$$\int_{-1}^{1} e^{i\rho\mu} P_l(\mu) d\mu = a_l \left[\frac{2}{2l+1} \right] j_l(\rho)$$
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So, let us see how to do that, so this is your e to the i k dot r, I have written k r as rho and cosine theta as mu, so as theta goes from 0 to pi, cos theta will go from 1 to minus 1, so mu will go from minus 1 to 1. So, to get this coefficient obviously, you can use orthogonality of the Legendre polynomials, so multiply this expression by a Legendre polynomial for some other value of l, here l is the dummy index which goes from 0 to infinity. So, multiply the left hand side by Legendre polynomial for l prime which is some particular value of l and now, I can use the orthogonality relation of the Legendre polynomial.

So, you evaluate this integral, here you have got the orthogonality, so there is a delta l prime l and this comes from the property of the Legendre polynomial. So, you have got 2 over 2 l prime plus 1, and now to get this coefficient what you need is this integral. So, if you can solve this integral the left-hand side, then you would know what is the value of a, a l that is your question. So, let us drop the prime, because you do not need it any more, so this is your relationship you need the prime only to distinguish it, from some other value of l. But, since that is already taken care of by the chronicle delta in the orthogonality relation, so this equation if you solve, you will be able to find what is a l.

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

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

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

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

$$P_{l}(\mu=1) = 1$$

$$P_{l}(\mu=-1) = (-1)^{l} P_{l}(\mu=1) = (-1)^{l}$$

$$P_{l}(\mu = 1) = \frac{1}{i\rho} \int_{-1}^{+1} P_{l}(\mu) e^{i\rho\mu} d\mu$$
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So, this is the integral to be evaluated and this is an integral over mu, this is an integral of a product of two functions, e to the i rho mu is one function, p l mu is another function, so this is just an integral of a product of two functions. So, I take p l mu as the first functions and e to the i rho mu as the second function, and use the usual formula which you would have used billions of times, in solving the integration of a product of two functions. So, you get p l mu e to the i rho mu over i rho between the limits minus 1 and plus 1, then you get you have to subtract from this, the integral of the derivative of the first function, which is d p by d mu.

And the integral of the second function which is e to the i rho mu over i rho, so now it is really very simple, because you can put these limits you can put mu equal to 1 and mu equal to minus 1. So, here in the first term I put mu equal to 1, in the second term I take mu equal to minus 1, I subtract the second term from the first term, so here is the minus sign, and then there is a residual integration to be carried out. Now, what will the residual integration give you, you already have a factor of 1 over rho here, here again you can carry out the integration by parts.

And when you do this integration by parts, once again you will get the integral of e to the i rho mu, which is e to the i rho, mu divided by i rho, so that together with this rho which you already have will give you a 1 over rho square. And that term will be much weaker than the terms which go as 1 over to rho in the asymptotic limit, that is the region of impressed.

Because, all this is being done to relate your results to your measurements, which are being carried out far away from the target.

And the meaning of far away from the target that is the question Lama asked me, at the beginning of this class as to what exactly is implied by this situation, that you should have the measurements sufficiently far away. See this scattering potential V of r will have a certain range, it could have an infinite range like the coulomb problem, the coulomb potential is goes as 1 over r and it goes to 0, only as r goes to infinity. You could have a potential which goes as 1 over r square, that will also go to 0 only as r tends to infinity and at any finite distance it will not be 0, but then it goes to 0 faster than the coulomb potential.

So, the question is at what rate does this potential go to 0 as r goes to infinity in the asymptotic region, and these are some questions of importance in this analysis. So, I will be discussing specific aspects of this condition as at what rate should this potential drop as r tends to infinity in the next class. But, I will give you some examples of finite range potentials, you can have spherical well for example, that the potential is like minus V 0 for r going from 0 to r 0 beyond this radius the potential can be 0, this is like a spherical value, it is like a cavity.

So, the region of influence has got a certain range and the detector must be well away from this range, if the detector is within this range then of course, you would not have examined the full consequence of the potential. So, that would beat the very purpose of measurement, now in a real experiment, in a physical experiment it is not that you really have to keep these detectors at infinity, then you cannot do the experiment. You have to do this experiment in a laboratory and most physical potentials of interest, they have got the certain range which is of the order of in some cases centimeters, in some cases meters and so on.

So, within a laboratory you do these experiments and that is the region of interest, which is where you can say that you are referring to r tending infinity by this asymptotic region. So, this term this integral in the range rho going to infinity will contribute, almost nothing compared to the 1 over rho terms, so these two terms are the Legendre polynomials, when the argument is 1 which is equal to 1, no matter what the value of 1 is. And when this argument is minus 1 this is it has a parody of 1, so it will be minus 1 to the 1, no matter what the value of 1 is.

So, these two Legendre polynomial's and this will give you e to the i rho over i rho, because P l of mu is equal to 1, in the second term P l of mu is minus 1 to the l. So, you get minus 1 to the l times e to the minus i rho over i rho and then you have got this integral which we know already will make ignorable contribution.

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

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

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

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

$$e^{il\alpha} = (e^{i\alpha})^l = (-1)^l$$
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So, this is the contribution which is of the order of 1 over rho square, so you can ignore this in all subsequent analysis, and this is now your solution, now this the what we needed to get the coefficient a 1. So, we already had a relation for a 1, which was given in terms of this integral and this integral we have now determined. So, now, the left hand sides are the same, the right hand sides would be the same, so you equate them and find what a 1 is. So, what does it give you for a 1, so you equate the hand sides and you get this you make use of the fact that e to the i 1 pi can be written as minus 1 to the 1.

So, this minus 1 to the l can be written as e to the i l pi and then you can combine it with this e to the minus i rho; so using this minus 1 to l, which is equal to the e to the i l pi, this is now your relationship between the left hand side and the hand side.

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

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

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

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

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

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And this will give you what the coefficient a l is, now you can write this in a slightly different form again and this is of some interest in our analysis, you will see why this manipulation of terms is useful. You can write this e to the i l pi as a product of e to the i l pi by 2 and e to the i l phi by 2, and then take e to the i l pi by 2 as a common term and pull it outside factor it out of the bracket. Because, then you get the arguments of both of these functions to be the same with the change in sign.

So, it is not something that you really want to remember, but these if you follow what is being done, you can automatically figure out how to proceed in this analysis. So, this is the advantage in factoring out this e to the ilp iby 2 and now you can write this solution, by looking at this you have got e to the i theta minus e to the minus it heta, so you will get the sinusoidal function out of it.

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

$$Now, \quad j_{l}(\rho) = \frac{\sin\left(\rho-\frac{l\pi}{2}\right)}{\rho} \qquad \Rightarrow a_{l} = i^{l}\left(2l+1\right)$$

$$e^{i\rho\mu} = \sum_{l=0}^{\infty} a_{l}P_{l}(\mu)j_{l}(\rho) \qquad \text{We got } a_{l} \text{ from } \rho \to \infty, \text{ but it is valid for all } \rho \text{ since } a_{l} \neq fn(\rho).$$

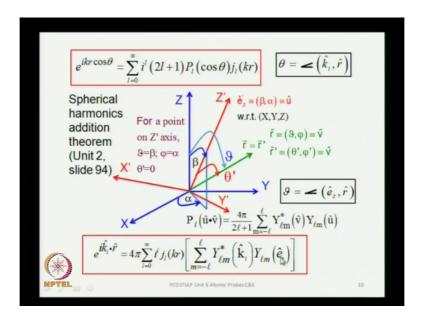
$$\Rightarrow e^{i\rho\mu} = \sum_{l=0}^{\infty} i^{l}\left(2l+1\right)P_{l}(\mu)j_{l}(\rho)$$

$$i.e. \qquad e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^{l}\left(2l+1\right)P_{l}(\cos\theta)j_{l}(kr)$$

And now you have got a very simple relation, which is emerging from this analysis that you do have spherical Bessel functions here, but these spherical Bessel functions also they are asymptotic forms. So, what is the asymptotic form of the spherical Bessel function, it is the same as the function of the sin, it is sin of rho minus 1 phi by 2 over rho. So, these are well known properties of special functions of the spherical Bessel functions and you can use this to get read of this sinusoidal function, you also get rid of the 1 over rho, which is common to both sides and it gives you a very simple result for your coefficient a l.

So, now you know precisely what the coefficients a l are, in the expansion of the plain wave, now of course, this solution is valid for the asymptotic region, but that is what we are interested in. So, these coefficients have now been determined this a l is i to the l 2 l plus l and then you have got the Legendre polynomial and the spherical Bessel functions, you can write in terms of k r and cosine theta.

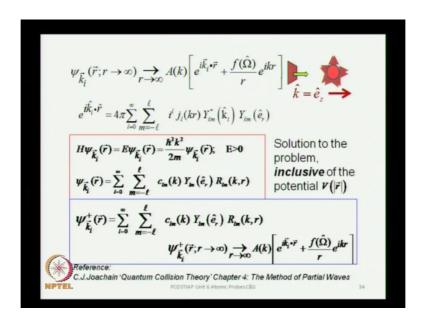
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And I will now make use of the addition theorem for spherical harmonics, which we did in unit 2, because this allows us to write this Legendre polynomial P I cos theta, this is the spherical harmonics addition theorem, which we have already discussed in unit 2, so this Legendre polynomial for an arbitrary value of I for an arbitrary angular separation between two directions U and V. This is given by the summation over a product of spherical harmonics, and you can plug in this summation in place of P I cos theta, so that you can write this plain wave e to the i k dot r or e i k r cosine theta.

So, here I have added a subscript here to the incident wave vector, just to keep track of the direction, because then the directions of these two spherical harmonic, the arguments of these two spherical harmonics are respectively. This unit vector along the direction of incidents, this is and then this is the radial unit direction, unit vector along the radial direction.

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So, these are various forms in which you can write the incident plain wave, this is the solution which represents the plain wave along with the coefficients, there are no unknowns now. The j l k r is also know that is the spherical Bessel function, you know it is asymptotic behavior with a sign of k r minus l phi by 2 divided by k r, so there is nothing that is not known over here and this part of the solution e to the i k dot r. The net solution is the super position of the incident wave plus the scattered wave, of which this part is now completely known.

((Refer Time: 28:31)) This solution must agree with the solution to the complete quantum mechanical problem, which is H psi equal to E psi, E is h cross square k square over 2 m for positive energies. And for this you will have a solution, which again you can write in terms of spherical harmonics and the radial solutions. But, with new coefficient c and these are now the unknowns of the problems, now how will you know that, it is now a very simple process. Because, you have got a solution in terms of the spherical harmonics and the radial functions.

These radial functions are known I mentioned earlier, but these are the same as the sinusoidal functions, but the phase shift is not just k r minus 1 pi by 2, this will be k r minus 1 pi by 2 plus a scattering phase shift. So, we will plug in that information and then from the difference between this and the plain wave or by matching the coefficients, you will get the exact seas which are the unknown coefficients.

So, that is what I mentioned towards the beginning of this class, that the only important mathematical idea over here, is that you have got an expansion of a wave function in a complete basis set. And when you have two alternative expressions, then the coefficients of the corresponding base functions must be equal, so that is it. So, let us proceed to do it, so I now add a super script plus over here, this will be of some importance in our subsequent discussion

Because, this is a solution to the scattering problem with what we will begin to call as outgoing wave boundary condition, what we are representing over here, is the scattering phenomenon in which the incident direction of the projectile that is fixed, that is the unique entrance channel. The outgoing waves go in all directions, in photoionization it is the other way around, and there you will find that this process is related to the scattering process, through the time reversal symmetry, which I will be discussing later.

And those solutions will come from what are known as in going wave boundary conditions, for which I will use the superscript minus over here. So, it is an anticipation of that, that I have started using psi plus, so keep that in your mind it will become important as we discuss the photoionization boundary conditions and then the whole picture will hang together nicely. So, here you have got this coefficients c 1 m of k, so this is expanded in a basis set of spherical harmonics.

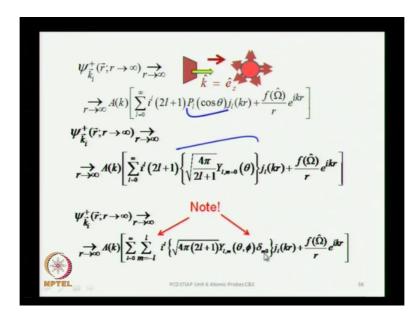
And these two solutions, one is ((Refer Time: 31:47)) this representation and the other is phenomenological solutions. These two solutions are essentially the same, then express the same mathematical solution to your quantum mechanical problem, and this is what you exploit to compare the coefficients of corresponding base functions.

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$$\begin{split} \boldsymbol{\psi}_{\vec{k}_{l}}^{+}(\vec{r}) &= \sum_{l=0}^{\infty} \sum_{m=-\ell}^{\ell} c_{lm}(k) \ Y_{lm}(\hat{e}_{r}) \ R_{lm}(k,r) \\ \boldsymbol{\psi}_{\vec{k}_{l}}^{+}(\vec{r};r \to \infty) \underset{r \to \infty}{\longrightarrow} A(k) \bigg[e^{i\vec{k}_{l} \cdot \vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr} \bigg] \\ e^{ikr\cos\theta} &= \sum_{l=0}^{\infty} i^{l} (2l+1) P_{l}(\cos\theta) j_{l}(kr) \\ \boldsymbol{\psi}_{\vec{k}_{l}}^{+}(\vec{r};r \to \infty) \underset{r \to \infty}{\longrightarrow} \\ \boldsymbol{\psi}_{r \to \infty}^{+} A(k) \bigg[\sum_{l=0}^{\infty} i^{l} (2l+1) P_{l}(\cos\theta) j_{l}(kr) + \frac{f(\hat{\Omega})}{r} e^{ikr} \bigg] \end{split}$$

So, now in this phenomenological solution, what the plain wave is it has got the expansion in the Legendre polynomials. So, you can insert this expansion over here, the second term is f of omega over r e to the i k r which comes here; the plain wave has now been expanded in the basis of Legendre polynomials.

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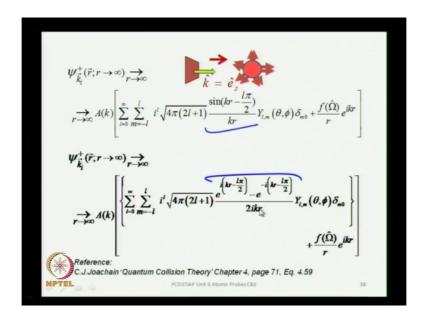


I bring it to the top of this slide and this Legendre polynomial, P l cosine theta can be written in terms of the spherical harmonic m equal to 0. And what this allows me to do is to write this summation over l going from 0 to infinity, I can add to that a summation over m going from

minus 1 to plus 1, just to get the complete basis. But, then I incorporate a delta m 0 chronicle delta here, because the only term that will contribute is the m equal to 0, which is a Legendre polynomial P1 cos theta, so I know what it is.

So, that is the only term that will contribute, so this summation which was only in terms of 1 can be written in terms of summation over 1, as well as summation over m, with m going from minus 1 to plus 1. So, you have got the complete basis set of the spherical harmonics, but then you already know that only the term for m equal to 0 and that is contained over here, there is a chronicle delta which has been included.

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So, this is the chronicle delta, which keeps track of the contraction over the summation over m, so that only the term in m equal to 0 has to be taken into account. You also know the asymptotic behavior of the spherical Bessel function, what is that, that is sine k r minus l phi by 2 over k r. So, the rest of the terms are written just as they were. So, this spherical Bessel function is now written explicitly for the asymptotic region are tending to infinity a sin of k r minus l phi by 2 over k r and then this is the scattered part which is e to the i k r over r multiplied by this scattering amplitude f of omega.

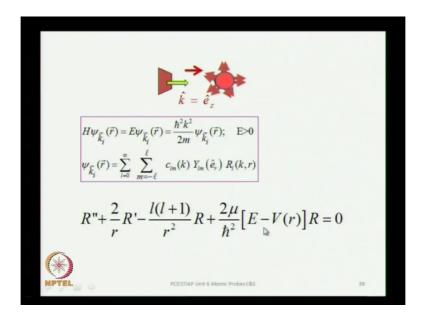
So, when you really sit down to write these terms one by one, sometimes one forgets one term or the other instead of this root of 4 phi 2 l plus 1 you miss out on some factor, so it is a little laborious, but if you do it carefully, it is not at all difficult. So, here you are, you have got this expansion, now the sinusoidal function you can write in terms of spherical outgoing

waves and spherical ingoing waves. Because, the sinusoidal function is something that you want to compare later on, you have to combine all of these terms, and this is made up of spherical ingoing waves as well as outgoing waves.

Those with the coefficient e to the i k r are the ones which corresponds to the outgoing wave, the one with coefficient which is the coefficient of e to the minus i k r, then it will correspond to the ingoing waves. Because, argument over there will be k r, the complete argument of the exponential function will be k r plus omega t, so the surface of constant phase will be converging to the centre in one case, and it will be diverging from the centre in the other. So, you have got two waves over there, two spherical waves one spherical in going waves and spherical outgoing waves.

So, this sinusoidal function you write in terms of spherical outgoing waves, and spherical ingoing wave by using this simple mathematical transformation, which we have used earlier, it is the same transformation. Everything else is the same, it is only the sinusoidal function which is written in terms of this spherical outgoing and spherical ingoing waves, the denominator is the same which is k r. The 2 i comes when you convert the sine function into the sum of these two exponential functions, so that is the twice i k r, that is how to get that twice i k r in the denominator.

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Now, let us look at the solution to the quantum mechanical H psi equal to E psi problem, this again you can break into the radial part and the angular part. The angular part which gives

you the solutions which are the spherical harmonics those are known; the radial part for each 1 will be a solution to the radial Schrodinger equation. This is the one that we have been discussed, so the radial part this one is a solution to this radio Schrodinger equation.

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

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

$$R_{d}(r) = \frac{y_{d(r)}}{r}; \quad U(r) = \frac{2mV(r)}{\hbar^2}$$

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

$$y_{l}(k,r) \xrightarrow{r \to \infty} A_{l}(k) \sin \left[kr - \frac{l\pi}{2} + \delta_{l}(k)\right]$$

$$R_{l}(k,r) \xrightarrow{r \to \infty} A_{l}(k) \frac{\sin \left[kr - \frac{l\pi}{2} + \delta_{l}(k)\right]}{r}$$

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You can write this differential equation for y instead of R in which we define this radial function as y over r that gives you a differential equation for y. Now, this differential equation for y can be solved you can simplify this by changing the units, you can introduce, you can multiply everything by minus of 2 m over h cross square. Then the potential gets multiplied by that V r are multiplied by 2 m over h cross square, so you call this scaled potential which is scaled by the constants 2 m over h cross square is just a constant scaling factors, so this is a scaled potential, which is sometimes called as a reduced potential.

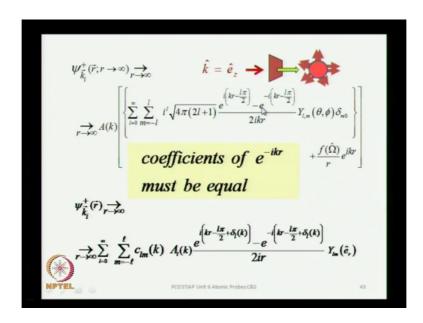
This only make writing the equation little easy, so that you do not write too many extra terms every time that is the only purpose of doing it, it is the same differential equation there is nothing new in it. So, now, you have got an equation which looks a little neater for some strange reason, it might give you a feeling that this is easier to solve than this. And in fact it is, it is not at all difficult to solve this is the same solution as you had earlier without the potential, we have already solve this problem exactly for 0 potential.

And the only thing that changes, when you have a potential which is what I mention and the conditions under which this works, there are some physical conditions on the potential which I will be discussing in the next class. That those conditions are on the rated with the potential

are formed as r tends to infinity. You got the solution which is the same as the sinusoidal function, and the only differences that argument k r minus l phi by 2 is phase shifted by this scattering phase shift, now this is the only difference.

And the solution for the radial function itself which is this function divided by r here it is, so you have got the 1 over r, this a normalization for which depends on 1 and k parametrical it is a independent of r. But, it will depend parametrically on the energy and it will be different for every orbital angle momentum quantum number.

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So, you have got the solutions now, this is the representation of the plain wave in the phenomenological solution, we want to find what are these coefficients. And now, we can easily do it because you have got an equivalent solution for this and you have got spherical outgoing waves over here and here and here. And you have spherical outgoing waves and ingoing waves in these two terms. So, now, if you compare the coefficients of the corresponding terms, you will be able to find what the coefficient c are, that is all the rest of it.

Because, the coefficient of the spherical ingoing wave must be the same in the both the representation, because the only thing that is going in, is completely represented in the component of the plain wave, which is incident, that is the only thing which is contributing to the ingoing waves. And that is explicitly determined already, because we found out what is the expansion of the plain wave in spherical harmonics, it had those coefficients A l and we

have explicitly found out those coefficients. So, those are no longer unknowns of the problem, so that is the merit of this technique and that is the heart of this technique.

So, you have these two expansions and you now equate the coefficients of the spherical ingoing wave, these coefficients must be exactly equal, so both are expansions over the complete basis sets. So, I goes from 0 to infinity n goes from minus I to plus I, now this is the advantage we got by going over from Legendre polynomials to this spherical harmonics, including this chronicle delta. Because, that is the only thing that we needed, but now we can compare the coefficients of the corresponding base functions.

So, now this part has got only an outgoing wave, so the only thing which has got an ingoing wave is over here, e to the minus i k r and what is the coefficient of e to the minus i k r, what will go into this coefficient.

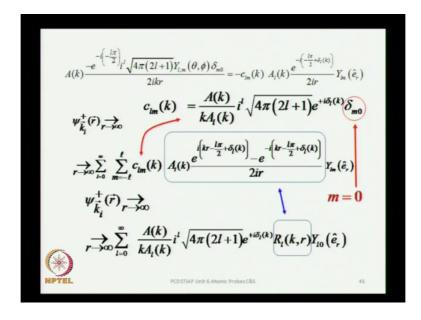
Student: ((Refer Time: 43:16))

i to the 1 will go in, root of 4 phi 2 1 plus 1 will go in, then e to the plus i 1 phi by 2 will go in, this y 1 m will go in and this chronicle delta will also go in, what about here ((Refer Time: 43:38)). So, here you will have the c, you will have the A and then you will have the e to the i 1 phi by 2 with a plus sign, but there is a minus sign over here, so do not forget that. There will be an e to the minus i delta that will also go in, and there will be this spherical harmonic. And then of course, there is this denominator 2 i r over here and this denominator 2 i k r over here, so you already identified the terms; now it is just a matter of writing it out carefully.

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So, this is the coefficient of e to the i k r, we already went through these terms and then over here this is the coefficient of e to the minus i k r in this expression. And now all you have to do is to equate this thing, which is in the yellow background with this thing which is in the blue background. If you just equate these two terms you will get the coefficient c, in terms of everything else; the missing things will be the normalizations A k and the A l k those are still unknowns. So, that is something that we can figure out how to deal with that, but everything else is known.

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So, we have now equated those two expressions and by equating them you get the c in terms of all the other factors, which is in terms of this phase shift, which is the one which has got information about the scattering potentials. Then there are these normalization constants A k and A l k and then everything else is known the only thing which is not known is of course, is the phase shift and by studying it you will get information about the target potential.

So, here you have this result that these coefficients are now determined and you can use these coefficients, which have now been determined over here. So, plug in this expansion, this expression for c 1 m over here, this function is nothing but the radial function which is the solution to the radial part. So, this ((Refer Time: 46:17)) gives you the complete expression for the scattering problem.

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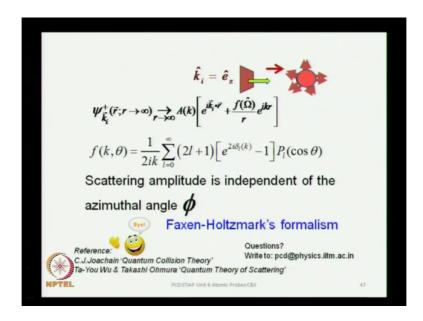
$$\begin{split} & \psi_{\vec{k}_l}^+(\vec{r};r\to\infty) \underset{r\to\infty}{\longrightarrow} \\ & \xrightarrow[l=0]{} A(k) \Biggl[\sum_{l=0}^\infty i^l (2l+1) \frac{e^{\left(kr-\frac{l\pi}{2}\right)} - e^{-\left(kr-\frac{l\pi}{2}\right)}}{2ikr} P_l(\cos\theta) + \frac{f(\hat{\Omega})}{r} e^{ikr} \Biggr] \\ & \psi_{\vec{k}_l}^+(\vec{r}) \underset{r\to\infty}{\longrightarrow} \sum_{l=0}^\infty \sum_{m=-\ell}^\ell c_{lm}(k) \ A_l(k) \frac{e^{\left(kr-\frac{l\pi}{2}+\delta_l(k)\right)} - e^{-\left(kr-\frac{l\pi}{2}+\delta_l(k)\right)}}{2ir} Y_{lm}(\hat{e}_r) \\ & \xrightarrow[must\ be\ equal \ } \\ & \underbrace{C_{lm}(k)}_{lm} = \frac{A(k)}{kA_l(k)} i \sqrt{4\pi \left(2l+1\right)} e^{+i\delta_l(k)} \delta_{m0} \end{split}$$

And what does it give you, the coefficients of the e to the plus i k r there must also be and when you want to relate them, the unknowns which are still sitting in the problem c, we have just determined that. So, we can use that value of c to compare the coefficients of the spherical outgoing parts, what will it give you, it will give you the only unknown in the outgoing wave component. This is the outgoing wave component the scattered solution, the only unknown over here is the scattering amplitude.

So, the scattering amplitude will, then be given in terms of these coefficients and what is sitting in these coefficients are the scattering phase shifts. So, the scattering amplitude will then be given in terms of the scattering phase shifts, by comparing these coefficients of the

outgoing wave, in which we have used this solution to the coefficient c, which we already obtained in the previous step.

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And by doing this analysis you get the scattering amplitude, in terms of the scattering phase shift, and this is simply by comparing the coefficients of the corresponding terms. Only the coefficients of the spherical outgoing wave, they must be exactly equal this is a very important result in scattering theory, this is sometimes called is the Faxen-Holtzmarks formalism. And it gives the scattering amplitude it is obviously, independent of the azimuthal angle phi.

And I will proceed from here in the next class is there any questions today, I will of course, be happy to take yes, any question.

Student: From intensity, what we get after scattering we will get intensity pattern or theta, so from it...

You take the scattering amplitude in different directions, so that gives you the differential cross section, what essential it is a measure, because the scattering amplitude will give you a physical quantity, whose modulus square will be proportional to the probability. So, it will give you the probability of scattering in a given angle, so the probability is not necessarily the same in all the directions, but it will be different in different directions and how does it

depend on this direction, how does it depend on theta, which is why it is called as a differential cross section.

So, you have got a total cross section sigma and d sigma by d omega, where d omega is a solid angle that gives you the differential cross section in a given direction. So, this angular distribution is what you get from this expression, that how is this intensity of scattering or the probability of scattering, is it uniform in all directions and if it is not uniform what is its angular distribution. So, that is the physical quantity of interest and that is what you are going to measure, these two references which I have mentioned over here.

These are very good sources Joachain quantum collision theory and quantum theory of scattering by Wu and Ohmura both of these are excellent sources. But, you will find this discussion in many books on quantum mechanics, Lyondell and Lifschitz is also a very good source and I have certainly taken some material from Lyondell and Lifschitz, so these are some references that you might want to use, any other question?

Student: ((Refer Time: 50:28))

Because, it is energy dependent, you have no reason to assume that this phase shift will be the same at all energies, k is the measure of the energy of the projectile, h cross square k square by 2 m is the energy. So, for different energies the phase shift that angle is not the same, so the phase shift depends parametrically on 1 quantum number and it is the function of the energy, that is the reason it has been written explicitly as a function of k. The whole problem is setup for a given energy H psi equal to E psi.

So, e is pin down you are solving this problem for a particular energy, when you solve the same problem for a different energy the solutions, we have phase shifts which are slightly different. So, when you do this energy dependence it is like doing spectroscopy at different wave lengths or different frequencies or different energies. So, when you study this phenomenon over a range of energy, you get an energy dependence which is contained in the scattering phase shift, which explicitly depends on the incident energy. And therefore, on the parameter k, so it is a function of k and it depends parametrically on the l quantum number, any other question.

So thank you very much.