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

Lecture 08 **Reciprocity Theorem, Phase Shift analysis**

Greetings, we will discuss the Reciprocity theorem today. We did the optical theorem in our previous class of course we have talked about the optical theorem earlier as well. And we have seen its connection with the unitarity of the scattering operator the conservation of flux. And we will go beyond the reciprocity theorem.

And pick up our discussion on the analysis of phase shift, scattering phase shifts. Because we know that they are intimately connected to the target potential and they contain the physical information about the target potential. (Refer Slide Time: 00:57)

 $\hat{f} F(\hat{n}') = \frac{1}{4\pi} \iint f(\hat{n}\hat{n}')F(\hat{n})dO \qquad \hat{S} = \left[1 + 2ki\,\hat{f}\,\right]$ Scattering Operator (definition) $\Psi(\vec{r}) \underset{r \to \infty}{\longrightarrow} \frac{e^{-ikr}}{r} F(-\hat{n}') - \frac{e^{ikr}}{r} \hat{S} F(\hat{n}')$ $\Psi(\vec{r},t) \underset{r \to \infty}{\longrightarrow} \frac{e^{-ikr}e^{-i\omega t}}{r} F(-\hat{n}') - \frac{e^{ikr}e^{-i\omega t}}{r} \hat{S} F(\hat{n}')$

 $\Psi(\vec{r},t) \underset{r \to \infty}{\longrightarrow} \frac{e^{-i(kr+\alpha t)}}{r} F(-\hat{n}') - \frac{e^{+i(kr-\alpha t)}}{r} \hat{S} F(\hat{n}')$ So, the expression for the scattering operator that we used in our previous class is this that the

scattering operator was defined as 1 + 2ki times the operator f where f was defined through this relation. It operates on a function of a direction okay; n prime is a direction unit vector. It picks a certain direction in space and you generate this integral from this operation so that is the definition of the f operator.

Now in terms of this we wrote the total wave function to the scattering problem as a superposition of in going waves e to the -ikr and outgoing wave's e to the ikr and you can combine these two terms. To write it in this form in which the scattering operator appears explicitly and its effect is what is included in the coefficient of the outgoing spherical waves.

And therefore it gives you information about scattering because that is where the scattering amplitudes right.

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So, this is the expression that we have for the total wave function. Now let us play with this a little bit do a complex conjugation first okay. We pick the scattering solution get its complex conjugate and notice that –i here goes to +i, F goes to F star this +i goes to –i. The scattering operator goes to S adjoint right and this F goes to F star okay.

So, all we have done here is the complex conjugation of the scattering wave function. The next thing, as some of you might anticipate is let t go to - t okay. So, you have got a plus omega t here which goes to - omega t and there is a - omega t here which goes to + omega t. So, this is this solution that you get on complex conjugation. (Refer Slide Time: 03:30)



And time reversal and the time reverse function is what we have written over here. And we now look at the space part of the time reversed function. This is the time reversal symmetry that we have discussed earlier in other context right. And we know from our discussion in our previous course and those lecture notes and even the video lecture is available you have the reference.

The, whenever you deal with time reversal in quantum mechanics you need to engage complex conjugation as well as t going to -t, the two things go together. So, that is exactly what we have done and we now extract just the space part of the time reverse function. So, let us study the space part of the time reverse function. So, this whole thing is a multiplied by e to the -i omega t and if you leave that factor out the rest of it is over here in the space part. (Refer Slide Time: 04:36)



So, this is the space part of the time reversed function and if you focus your attention on this term here which is S star operating on F star okay. How did we get this S star it came from the complex conjugation step right. So, you have the S star operating on F star and we now introduce a new function Phi by using this definition of Phi function.

Phi function is so defined that S star Phi star = - Phi with an argument in which the direction of the unit vector is reversed okay. This is the definition of Phi okay. So, now this is your F star n star and you will preserve this relation if you pre operate on this by a unit operator which I resolve as S star inverse S star okay.

S star is the complex conjugate operator. So, I pre operate on this function by the unit operator resolved as such. And now we make use of this definition here because F star n prime when you operate on this by S star you get - Phi times - Phi with the argument - n prime. So, this is the one that you find from this part alone S star operating on F star. And now you have got the S start inverse operating on it okay.

This is very simple operator algebra but it is going to give us some very exciting results. So, what is this equal to S star inverse is what you have; you just have the minus sign brought out okay. So, you got minus of S star inverse operating on Phi of - n prime but this is the inverse of a certain operator coming out of the scattering operator. And you know that the scattering operator is unitary.

So, this relation is completely equivalent to - S star adjoint operating on this right. What we have used over here and going from this step to this step is the unitarity of the scattering operator which we have established in the previous class. So, now we have got the unitary operator you already have S star over here and in this adjoint, what does an adjoint do? It does transposition and complex conjugation right.

So, in this process of taking the adjoint of this operator you will have the complex conjugation as well as transposition. So, the complex conjugation will sort of undo the complex conjugation indicated by this asterisk over here and you will be left with the transposition alone which is indicated by this tilde on top of this operator okay. So, the tilde is the complex conjugation, so S star adjoint is s tilde okay, tilda stands for transposition.

So, now consider the parity operator what does the parity do it will reverse the direction of the argument okay. So, here if you have got a direction, this direction is reversed by parity right. So, parity operating on F star n prime would give you F star - n Prime. So, what is F star n prime, F star n prime is over here it is - Phi times Phi of - n prime. So, that is the term, you right over here, fair enough.

And if you now recognize that you have got - n prime that this is something that will result by the operation of the parity on Phi because that is precisely what parity will do to this direction, it will reverse it. So, now you have got another result here that F star - n prime is =

- PS tilde P operating on Phi. (Refer Slide Time: 09:31)

space part of the time-reversed function: $= -P\hat{S} \left[P\Phi(\hat{n}') \right]$ PSPO(n space part of the time-reversed function: $\widehat{S}^* F^*(\widehat{n})$ $\widehat{S}^* F^*(\widehat{n}') = -\Phi(-\widehat{n}') \rightarrow \text{definition of } -\Phi(-\widehat{n}')$ space part of the time-reversed function:

So, let us carry this result to the top of the next slide here. So, this is the result which we have recovered that F star - n prime = - P S tilde P operating on Phi. This is the space part of the time reverse function in which you have got F star this term over here. But this we have found to be equal to this.

So, what we can do is replace this term by its equivalent term on the right hand side and write this term, rewrite this term as - P S tilde P operating on Phi okay good. Now what about this S star F star operating on n prime is using the definition, we already have this result which is - Phi up with an argument - n prime okay.

This is the original definition of the function phi. So, using this definition we can replace this term in terms of Phi. So, replacing this term S star operating on F star using the definition of Phi we replace this term by -Phi -n prime and what is this? This is the space part of the time reversed function okay. (Refer Slide Time: 10:58)



So, the space part of the time reverse function is now written in terms of the function Phi we started out with the function f. But now we have it in terms of the function Phi everything is in terms of function phi. And I just write, just for convenience the ingoing wave terms first and the outgoing above wave term next.

So, there is nothing new in this relation which is not there in the previous one except that I have written the second term first and the first term second. Because that makes it easy for me to compare this form with how we had it in the original function. In the original function we had the ingoing wave term first, so now if you look at this comparison okay. What have we done? We have just done a little bit of you know simple mathematics.

We have not operated on the function by some other physical operators and change the state of the system and so on. So, you are essentially talking about the same physical state of the system but written differently now. It is exactly the same thing that you started out with which means that these functions Phi and F these are this is only a matter of notation.

Because we have not done any operation any physical operation to change the state of the system, is the same physical state. But now written in terms of a different notation and since notation is not central to physics you can call a function as f, Phi, Psi, Xi whatever right. What is important that it is a certain function of a direction right? So, here the direction is n prime, here the direction is -n prime okay.

And these things you cannot tamper with. So, if you look at that here you have got a function of n prime here you have got a function of -n prime it is exactly the same. And if you now see the operator identity then the operator PSP must be exactly equal to this S but find you on this middle S there is a tilde okay, there is a transposition.

So, you get an operator identity that PS tilde P = S where S is the scattering operator S tilde is defined as its transposed operator okay. (Refer Slide Time: 13:50)



So, this is an operator identity that you get and if you now look at these pictures they are rather interesting. See that you have got a certain direction of incidence which is the unit vector n. There is a certain direction of scattering which is n prime. And we take away the polar axis which is the axis of reference to be the scattering direction okay.

Earlier on we had the incident direction as the direction reference direction for the polar axis. But when we consider the unitarity and the superposition coming in from the phenomenology being invariant if you construct a super position with respect to all different incident directions right then the reference direction considered was the scatter direction.

So, now you have the scattered direction indicated by n prime it could be any direction in space which is why I have drawn these arrows randomly it is some direction in space and then you have got this direction over here which is the direction of incidence. Now interchange the incidence direction and the scattered direction okay.

So, this direction is what did I now call as n prime and this is what I call as n. I have interchanged change n and n prime which amounts to interchanging the direction of incidence and the direction of scattering okay. Having done it the next thing we do is reverse the sign. You reverse the sign of the scattered direction, reverse the sign of the incident direction as well what have you done? You have reversed the motion right.

You have essentially reversed the motion which is why the time reversal operator should actually be called as motion reversal operator and that is the correct term. But the time reversal has come into vogue and we continue to use it. But essentially the process that we are discussing at the time reversal operation is this motion reversal which is what we have considered in these pictures.

And because of this motion reversal symmetry the time reversal symmetry that we talked about this operation S n prime if you interchange you get n prime first and n next and when you reverse the signs you get -n prime first and -n next and these must be exactly equal okay. This is very beautiful argument which gives you some insight into the motion reversal symmetry.

And this is straight out of Landau Lifschitz book Quantum Mechanics, The Non Relativistic Formulation and I strongly recommend that you refer to Landau Lipschitz book for this part. So, this is the motion reversal of the scattering process. (Refer Slide Time: 17:07)



What it essentially means that if you interchange the incidence and the scattered directions and reverse the signs you get this expression for the scattering operator. And what it results with respect to the scattering amplitudes that when you express the scattering amplitude defined in terms of what is the scattering amplitude a function of, it is a function of the angle.

And how do you measure this angle? You can measure it with reference to the direction of incidence how much has the scattered direction changed okay. That is the original definition of the angle that comes in the scattering amplitude. And now result is completely equivalent because of this relationship that you recover the scattering amplitude in which the incidence direction is - n prime and the scattered direction is - n right.

So, that is the result that you get which is known as the reciprocity theorem that the scattering amplitudes for two scattering processes which are time reversed processes of each other are exactly the same okay. So, this is allowed in quantum theory that if a particle come this way and get scattered this way then it could come this way get scattered this way and the corresponding scattering amplitude will be the same okay.

The scattering amplitude which is a measure of the probability of the process that is what you are interested in. So, what is the probability that a particle comes this way and get scattered in this way that probability is now exactly equal to the probability that it comes this way on the scattered particle goes this way right. So, this is the reciprocity theorem and this is also a very nice thing to learn it is an expression of motion reversal symmetry.





And essentially what time reversal does is interchanges the initial in the final states and reverses the direction of motion of the particles in those states okay. So, this is the time reversal symmetry in scattering phenomenology. (Refer Slide Time: 19:26)



And we have considered this earlier in the discussion of recognizing photo ionization as half scattering right. Which were also connected by time reversal symmetry the solutions were connected were recognized as time reversed solutions of each other. (Refer Slide Time: 19:45)



And this we have discussed in a different unit in the previous course. So, I will not repeat that

part of the discussion. (Refer Slide Time: 19:55)



And now we will consider the partial wave analysis in some further detail because we have been saying repeatedly that the objects of central interest in scattering theory are the phase shifts. The phase shifts are the one which contain information about the target potential right. So, if you look at the partial wave analysis.

Let us begin to see how to extract information about the potential from the phase shifts okay. We have only said that the phase shifts are generated by the target potential. But how do we get information about the potential from the phase shift. So, we are now getting into the details of phase shift analysis.

And we find that the total scattering cross section is now given by the sum of all these partial wave contributions. And we have obtained this expression earlier, so let us use it okay. And let us also use the fact that we used some semi classical arguments to show that you do not have to consider all the infinite partial waves but a certain maximum number is sufficient okay because of the centrifugal barrier effect.

Now consider the scattering phenomenon in which you do not have to consider a large number of partial waves that depends on the details of the target potential right. So, there may be a situation and indeed there are some situations I am going to give you an example of one of those.

In which you really do not have to consider a large number of partial ways you need to consider only one of them. Which is the lowest one l = 0, which is the case of s wave scattering okay, l = 0 is the s orbital right. So, these are the s wave's s partial waves and if s partial waves alone are involved in a certain scattering process you need to consider only one term.

So, the term that you are dealing with this sigma total is completely given by a single term on the right hand side which is sigma 0. And what is that sigma 0 = sigma 0 = 4 PI over k square, 21 will be equal to 0, because 1 = 0. So, 4pi by k squared times sine square delta is the contribution of the s wave to scattering cross section right.

Now what happens if this phase shift goes to n pi, if for l = 0, if the phase shift goes to n pi, sine of n pi vanishes. What does it do to the scattering cross section? 0, there will be no scattering, so you have a target; you have an incident beam but only s wave scattering is of interest in this case, you do see the scattering okay.

But what does the phase shift depend on? It also depends on k. So, only at a particular value of k v delta of k become equal to n pi, for lower values or higher values of k it will not be so right. So, there will be some energy and what is kh cross square k square by 2m is the energy, so k is going to change with the energy of the incident beam.

So, there will be some energies of the incident beam which will not be scattered by the target at all, whatever comes in will be seen on the right hand side on the other side of the target as if the target was completely transparent to the incoming beam and scattering cross section will vanish at those energies.

And this is what is called as a Ramsauer Townsend effect, so this is, if the electrons will come they will just go through the target this is called as our Ramsauer Townsend effect. And if you remember when we discuss some, one dimensional analogues of scattering I had mentioned this in even in one dimensional problems, you have this transmission coefficient and reflection coefficient and that shows some oscillations if you remember that.

But that is I do not want to get into one dimensional problem at this stage. So, the Ramsauer Townsend effect is you can see in various experiments this is the probability of scattering and it goes to a minimum it very nearly vanishes okay, does it quite go to zero because there may be some residual contribution from other partial waves okay, s wave scattering is the dominant one but there may be a little bit of contribution from some of the other ones.

So, it does not quite go to zero but it does go through a minimum. And this is the low energy scattering which was seen in rare gas atoms like Xenon, Krypton, Argon and so on. I would like to refer you to this very nice paper in the American Journal of physics by Kukolich, I do not know how exactly I should pronounce this name. But this is a very nice paper to read in the American Journal of physics.

And you see that it discusses the realization of Ramsauer Townsend effect in low energy Xenon scattering okay. So, this is a very nice quantum effect and this will have no classical analog at all because you have an incident beam which gets scattered. And then if you just change the energy and somehow the scattering vanishes like magic okay. So, this is what quantum mechanics does to physics. (Refer Slide Time: 26:12)

 $\psi_{inc} \underset{r \to \infty}{\overset{1}{\longrightarrow}} \frac{1}{2ikr} \sum_{l} (2l+1) \left[P_l(\cos\theta) e^{ikr} - P_l(\cos\theta) (-1)^l e^{-ikr} \right]$ $\psi_{\text{Tot}}\left(\vec{r}\right) \xrightarrow[r \to \infty]{} \left\{ c_l^+ = e^{i\delta_l(k)} \right\}$ $\frac{1}{2ikr}\sum_{l} (2l+1) \Big[P_l(\cos\theta) e^{ikr} e^{i2\delta_l(k)} - P_l(-\cos\theta) e^{-ikr} \Big]$ Phase shifts are caused by the scattering potential, so to study them we consider two different scattering potentials. PCD STITACS Unit 1 Quantum Theory of Colli 138

And we will now discuss the phase shifts further. So, you already see that the phase shift plays a very magical role and it is going to be generated by the potential. So, certain potentials will be capable of causing such effects because this, the disappearance of the cross section has come because of a particular property of the phase shifts. So, phase shifts play a essential role in collision physics.

So, we will study these phase shifts further and best way to study them will be to consider phase shifts caused by two different scattering potentials okay. To study how phase shift depends on potential we will consider two potentials and ask what will be the phase shift caused by one potential.

How does it compare with the phase shift caused by the other potential, is it the same, is it different. And if it is different, how do these two potentials differ from each other that is what will give us knowledge about the two potentials right. (Refer Slide Time: 27:29)

$$\begin{split} \mathbf{R}_{st}(r) &= \frac{y_{stry}}{r} \left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - U(r) \right] y_l(k,r) = 0 \quad \underbrace{U(r) = \frac{2mV(r)}{h^2}} \\ &= \underbrace{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - U(r) \right] y_l(k,r) = 0}_{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = 0} \\ &= \underbrace{U(r) = \frac{2mV(r)}{h^2}}_{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = 0} \\ &= \underbrace{U(r) = \frac{2mV(r)}{h^2}}_{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = 0} \\ &= \underbrace{U(r) = \frac{2mV(r)}{h^2}}_{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = 0} \\ &= \underbrace{U(r) = \frac{2mV(r)}{h^2}}_{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = 0} \\ &= \underbrace{U(r) = \frac{2mV(r)}{h^2}}_{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = 0} \\ &= \underbrace{U(r) = \frac{2mV(r)}{h^2}}_{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = 0} \\ &= \underbrace{U(r) = \frac{2mV(r)}{h^2}}_{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = 0} \\ &= \underbrace{U(r) = \frac{2mV(r)}{h^2}}_{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = 0} \\ &= \underbrace{U(r) = \frac{2mV(r)}{h^2}}_{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = 0} \\ &= \underbrace{U(r) = \frac{2mV(r)}{h^2}}_{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = 0} \\ &= \underbrace{U(r) = \frac{2mV(r)}{h^2}}_{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = \underbrace{U(r) = \frac{2mV(r)}{h^2}}_{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = \underbrace{U(r) = \frac{2mV(r)}{h^2}}_{\left[\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \overline{U}(r) \right] \overline{y}_l(k,r) = \underbrace{U(r) = \frac{l(l+1)}{h^2}}_{\left[\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac{l(l+1)}{r^2} - \frac{l(l+1)}{r^2} - \frac{l(l+1)}{r^2} + \underbrace{U(r) = \frac{l(l+1)}{h^2}} - \underbrace{U(r) = \frac{l(l+1)}{r^2}}_{\left[\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac$$

So, we will consider scattering by two potentials now and we are now dealing with a reduced potential which is just scaling by this 2m over h cross square which is to simplify our notation. We will also deal with the radial function written not as capital R but as y over r. So, that we consider the differential equation for the little y okay.

So, the radial equation for the Schrodinger equation you get by separating the angular part. And the radial part if you multiply my little r you get the y function and the differential equation that y must satisfy is this right. For the potential U and now if you are considering two different potentials there are two such equations one for U and the other for the other potential.

The second potential I am denoting by U bar, so there is a bar put on top of this U. So, there are two potentials one is U the other is U bar, these are the two potentials and their solutions are respectively y and y bar. So, these are the two functions which are solutions to the radial y equations. So, you can normalize them each potential will be responsible to generate a phase shift right which is why you get a phase shift delta from the first function.

And phase shift delta bar from the second function. So, we have used these relations earlier except that now we are using two of them okay. So, each of these equations we have seen earlier but now we are considering them as a pair, so that we see what is the relative difference between the phase shift caused by the potential U in comparison with the potential U bar.

So, this is the normalization you have got the phase shift because of the potential U and the phase shift delta bar caused by the potential U bar. (Refer Slide Time: 29:30)

$$\begin{bmatrix} \frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - U(r) \end{bmatrix} y_l(k,r) = 0 \\ \begin{bmatrix} \frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \overline{U}(r) \end{bmatrix} \overline{y}_l(k,r) = 0 \\ \times y_l(k,r) \end{bmatrix} \begin{bmatrix} \mathsf{Eq}.\mathsf{A} \\ \mathsf{Eq}.\mathsf{B} \end{bmatrix}$$

$$\begin{bmatrix} \mathsf{Eq}.\mathsf{A} - \mathsf{Eq}.\mathsf{B} \\ y_l^{\mathsf{T}}\overline{y}_l - \overline{y}_l^{\mathsf{T}}y_l - \left(U - \overline{U}\right)\overline{y}_ly_l = 0 \\ \end{bmatrix}$$

$$\begin{bmatrix} \mathsf{Eq}.\mathsf{A} - \mathsf{Eq}.\mathsf{B} \\ Wronskain of the two solutions \ y_l(k,r) \ and \ \overline{y}_l(k,r) \\ (definition): \\ W[y_l(k,r), \overline{y}_l(k,r)] = y_l(k,r)\overline{y}_l'(k,r) - \overline{y}_l(k,r)y_l'(k,r) \\ prime \rightarrow \text{derivative with respect to } r \\ \end{bmatrix}$$

$$\begin{bmatrix} -\frac{dW}{dr} - (U - \overline{U})\overline{y}_ly_l = 0 \\ -\frac{dW}{dr} = -(U - \overline{U})\overline{y}_ly_l \\ \frac{dW}{dr} = -(U - \overline{U})\overline{y}_ly_l \\ \end{bmatrix}$$

And these are the differential equations we are dealing with. And now let us do a little bit of simple mathematics with this take the first equation multiplied by y bar, take the second equation and multiply it by y call them as equations A and equation B after this multiplication.

And then subtract equation B from equation A okay. So, the product terms like k square y y bar and k square y bar y will cancel right. And the remaining terms will give you y double bar, y double prime, y double prime. Prime denotes derivative with respect to r okay. So, y double prime is d2y by dr2, so that is the result of this operation d2 by dr2 right.

So, you get y double prime y bar - y bar double prime y the term in which you have got multiplication by k square and this - 1 into 1 - 1 the centrifugal term they will cancel each other right. And then you will have these terms U - U bar and then y bar y make sure that you keep track of the sign correctly because you are doing a subtraction and there are some intrinsic minus signs okay.

So, if you just do it carefully this is an easy result to obtain and this result you can write in turn terms of the Wronskain okay. When you have two solutions y and y bar of a differential equation, the Wronskain is defined for these pair of functions y comma y bar as yy prime - y y bar prime - y bar y prime right. This is the usual definition of Wronskain in differential equations, differential calculus that you would have learned.

So, we will use this Wronskain, here again I am denoting by prime the derivative with respect to r. So, this is the definition of Wronskain and this relation you can now write in terms of Wronskain because these two terms are coming by taking the derivative of Wronskain. If you take the derivative of the Wronskain, if you take the derivative of the right hand side you get the first two terms as you can see very easily right.

You take the derivative of these two terms on the right hand side you get these two terms and this box in this red loop is now written over here okay. We are all together very good, so let us write it for dw by dr which is the derivative of Wronskain and you move this term to the right take care of the signs this is written for + dw by dr. So, this is - of U - U bar okay. So, all the signs are taken appropriately care of right. (Pafer Slide Time: 22:41)

(Refer Slide Time: 32:41)

$$\frac{dW}{dr} = -(U-\bar{U})\bar{y}_{l}y_{l}$$

$$\int_{r=a}^{r=b} \frac{dW}{dr} dr = -\int_{r=a}^{r=b} (U-\bar{U})\bar{y}_{l}y_{l}dr = -\int_{r=a}^{r=b} \bar{y}_{l}(U-\bar{U})y_{l}dr$$

$$W[y_{l}(k,r),\bar{y}_{l}(k,r)]_{a}^{b} = -\int_{r=a}^{r=b} \bar{y}_{l}(U-\bar{U})y_{l}dr$$

$$[y_{l}(k,r)\bar{y}_{l}'(k,r) - \bar{y}_{l}(k,r)y_{l}'(k,r)]_{r=a}^{r=b} = -\int_{r=a}^{r=b} \bar{y}_{l}(U-\bar{U})_{a}y_{l}dr$$

$$[y_{l}(k,r)\bar{y}_{l}'(k,r) - \bar{y}_{l}(k,r)y_{l}'(k,r)]_{r=0}^{r\to\infty} = -\int_{r=a}^{r\to\infty} \bar{y}_{l}(U-\bar{U})y_{l}dr$$

So, this is the relation that you are now working with what happens if you integrate this, left hand side is the total derivative of the Wronskain and integration and differentiation are inverse operations right. So, if you integrate the left hand side you will get Wronskain. So, let us integrate it between limits r = a to r = b. So, each term is integrated okay, the left hand side as well as the right hand side right.

Here I have only written this symmetrically it does not matter in what order you write these three terms okay. They are all multiplicative terms, so you have got U - U bar sandwich between these two just then it looks a little nicer and symmetric. And the integral of the left hand side which is the integration of a total derivative gives you the Wronskain itself.

And you have to subtract the value of the Wronskain at the lower limit which is a from the value of their own scale at the upper limit which is b. So, that is the result for the left hand side on the right hand side you have got this integral with a minus sign are going from a to b of this y bar U - U bar y dr. So, let us write this Wronskain this is the definition of the Wronskain.

Then we will have to consider the value of the difference of these two terms at the lower limit and subtract it from the corresponding value at the upper limit and this will be equal to the right hand side okay. And now a and b are any two values of r, so let us take r = 0 and let the upper limit go to infinity and let us see what we get from this. (Refer Slide Time: 34:54)



So, let us consider this relationship here bring it to the top of the slide. And now we need to consider the difference between these two but what we do know is at r = 0, the function is y as well as y bar go is r to the power l + 1 right. The radial function goes as r to the power l this is the radial function multiplied by little r. So, it goes as r to the power l + 1, so no matter what the value of l is including 0, this function y as r tends to 0 will go to 0.

So, the value of these terms at r = 0 vanishes right and you have to subscribe 0 from the value at the upper limit, so you really have to deal with only the value at the upper limit that is it which is in the asymptotic region which is good because we know the asymptotic solutions right. We certainly already know the solutions in the asymptotic region. So, let us write this expression for the asymptotic region.

And from the asymptotic region we know that the solutions are sum of the sine and cosine functions. And the cosine term is weighted by the tangent of the phase shift but the phase shift is delta for y, it is delta bar for y bar. So, you have got y and y bar in terms of delta and delta bar and you take this difference and you only need to consider the value at the upper limit which is r tending to infinity.

The value at 0 which you have to subtract is itself going to 0. So, you just have to subtract 0 from whatever you have at the upper limit in the asymptotic region. (Refer Slide Time: 36:37)

Evaluation in the asymptotic regio $-\int \overline{y}_l (U-\overline{U}) y_l dr$ $\left[y_l(k,r)\overline{y}_l'(k,r) - \overline{y}_l(k,r)y_l'(k,r)\right]$ sin kr $+\tan \delta_i(k)\cos kr$ $\sin\left(kr - \frac{l\pi}{2}\right) + \tan \overline{\delta}_{i}(k) \cos\left(kr\right)$ $y_{i}(k,r)_{\substack{r \to \infty}} \left[\cos\left(kr - \frac{l\pi}{2}\right) - \tan \bar{o}_{i}(k) \sin\left(kr - \frac{l\pi}{2}\right) \right]$ $\bar{y}_{i}(k,r)_{\substack{r \to \infty}} \left[\cos\left(kr - \frac{l\pi}{2}\right) + \tan \bar{o}_{i}(k) \sin\left(kr - \frac{l\pi}{2}\right) \right]$ 1st derivative $[y_l(k,r)\overline{y}_l(k,r)-\overline{y}_l(k,r)y_l(k,r)]$

So, you now have to evaluate the value of this difference in the asymptotic region. So, you must write the wave function y in the asymptotic region and given the function y you can take its derivative and get y prime. So, you need y prime over here and you need y bar prime to put over here.

But you have both y as well as y bar okay they differ only the respective phase shifts which are delta and delta bar. So, this is y and this is y bar both the solutions are known. This has got phase shift delta, this has got phase shift Delta bar. Then you need the derivatives, so you have the first derivative y bar you take the derivative of the sine function.

You will get k times cosine kr right, but there is a 1 over k sitting over here, so that will cancel the k, so this is the y bar and you have got a similar expression for y bar prime which is the derivative of y bar okay, quite easy. So, you have got the functions as well as the derivatives, so you multiply y by d by dr of y bar to get this and then you multiply y bar by this d by dr of y which is this.

So, you just have to cross multiply all of these terms to get the left hand side. So, what do you get you cross multiply, so all the terms have been written explicitly over here? This is y, this y is multiplied by y bar and from this you subtract y bar which is this which is going to multiply the derivative of y which is this okay. (Refer Slide Time: 38:39)

$$\begin{split} & \textbf{Frequencies} \\ & (y_{\ell}(k,r)\overline{y_{\ell}}(k,r) - \overline{y_{\ell}}(k,r)y_{\ell}(k,r)) \\ & (y_{\ell}(k,r)y_{\ell}(k,r) - \overline{y_{\ell}}(k,r)y_{\ell}(k,r)) \\ & (y_{\ell}(k,r)y_{\ell}(k,r) - \overline{y_{\ell}}(k,r)y_{\ell}(k,r)) \\ & (y_{\ell}(k,r)y_{\ell}(k,r) - \overline{y_{\ell}}(k,r)y_{\ell}(k,r)) \\ & (y_{\ell}(k,r)y_{\ell}(k,r)y_{\ell}(k,r)) \\ & (y_{\ell}(k,r)y_{\ell}(k,r)y_{\ell}(k,r)y_{\ell}(k,r)) \\ & (y_{\ell}(k,r)y_{\ell}(k,r)y_{\ell}(k,r)y_{\ell}(k,r)) \\ & (y_{\ell}(k,r)y_{\ell}(k,r)y_{\ell}(k,r)y_{\ell}(k,r)) \\ & (y_{\ell}(k,r)$$

So let us bring this to the top of the next slide this is what we have got right and we can simplify this a little bit I think in this I have not done much of simplification except that this 1 over k which multiplies this term as well as this term I have written outside this bracket. So, that I can extract it as a common factor okay, so this is a very minor rearrangement on this slide. So, with this minor rearrangement you have got 1 over k outside this bracket. (Refer Slide time: 39:22)



And these are the terms that you get seems messy but it is not it is exceptionally simple because if you look at the terms notice that this one cancels this because this one is with a plus 1 over k. This one is multiplied by - 1 over k okay. So, these are equal and opposite terms they will cancel each other right.

Then what do you have these terms cancel each other they are the same, you got the product of the sine and the cosine function and you have got the product of the two phase shifts tan delta and tan delta bar. You have got the same over here the sine function and the cosine function the tan delta and the tan bar. But then this one is with a minus sign multiplied by +1 over k. This one is with a minus sign but it is multiplied by -1 over K.

So, they have relatively opposite signs, so they cancel; now it is getting simpler. But it becomes even simpler. What do you have in the remaining terms, look at these two terms what do you have? Both have tan delta bar this is a minus sign right. This is also a minus sign. And in one you are multiplied by sine square of this angle. In the other you multiplied by cos square of the other angle.

So, you have tan delta bar multiplied by sine square theta $+ \cos$ square theta which = 1 right. So, that becomes simple and you have the same thing happening with the remaining term if you look at these terms this tan delta \cos square delta. And then this is the term which has got the phase shift delta without the bar.

So, if you combine these two terms you have got a similar simplification. So all this mess reduces to a very simple expression which is 1 over k times tan delta - tan delta bar okay this is tan delta - sine delta bar. (Refer Slide Time: 41:32)



And now you can write your result that for the asymptotic region the tan delta - tan delta bar divided k is equal to this integral or you can take k to the right hand side okay. Now y bar is a potential U bar which can be anything I can choose it to be whatever potential I want, I can choose it to be zero.

Which is also a spherically symmetric potential right as a special case of a spherically symmetric potential I take v = 0, so U bar becomes equal to 0 and that gives me an expression for tangent delta because tan delta bar now goes to 0 right, U bar being zero. So, tan delta is

now equal to -k times this integral 0 through infinity. What is y bar, this is the Bessel function that is the solution to the free electron case right.

Which we know is the spherical Bessel function multiplied by r right. And then you have got Ur U bar is 0 and this y is a solution to the problem in which v is not equal to 0. So, this is the expression for tan delta and you find that this expression is telling you explicitly how the phase shift delta depends on the potential U okay. This is what we have always been saying that the phase shift is determined by the potential.

And now you see exactly how, so this there is no approximation in this, this is exact but it is not terribly useful because you also need the solution r for v not equal to 0 and that solution also has the phase shift okay. So, this result is exact is not terribly useful but you can develop some approximations. So, this is the expression you get for the phase shift okay. And you have a little r over here; you have got a little r over here.

So, these two little r's give me an r square here, so the same integral I have rewritten but r square is now written over here okay that is for certain convenience and you know what the delta is coming from. It is coming from the fact that this potential is now not 0. So, the corresponding radial function will be a sum of the Bessel function and the Neumann function. The Neumann function will be weighted by the tangent of the phase shift okay. (Refer Slide Time: 44:24)

$$\tan \delta_{l}(k) = -k \int_{r=0}^{r \to \infty} j_{l}(k,r)U(r)R_{l}^{V \neq 0}(k,r)r^{2}dr$$

$$\tan \delta_{l}(k) = -\int_{r=0}^{r \to \infty} \{(kr) j_{l}(k,r)\}U(r)\{rR_{l}^{V \neq 0}(k,r)\}dr$$

$$rR_{kl}^{(\nu=0)}(r \to \infty) \to 2\{(kr) j_{l}(kr)\} \to \frac{r \to \infty}{asymptotic} 2\sin\left(kr - l\frac{\pi}{2}\right)$$

$$E > 0 \text{ continuum for } V = 0$$

$$\left[rR_{l}^{V \neq 0}(k,r) \xrightarrow{r \to \infty} \sin\left[kr - \frac{l\pi}{2} + \delta_{l}(k)\right]\right] \text{ Examine their nodal behavior}$$

So, here is this result and for v = 0 you know the solution it is the Bessel function. You know that this Bessel function in the asymptotic region goes as a sine function in which the argument kr is reduced by pi by 21 times depending on what the value of 1 is. And now I suggest that you now consider a comparison of the two solutions. These are the two solutions this is for v = 0 this is for v not equal to 0 that is our problem of interest.

How does the potential generate the phase shift and how do we get information about the potential from the phase shifts. So, you compare it with the situation when there is no potential. So, here there is no phase shift kr - 1 pi by 2, here you have got the same kind of solution with the phase shift delta. And ask where are the nodes of these functions when does this function go to 0 okay.

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So, these nodes when v is not equal to 0 are when this argument of the sine function kr - 1 pi by 2 + delta well this argument is equal 2m pi, you will have the nodes. In this case you will have the nodes when kr - 1 pi by 2 = n pi right. What does it tell you with reference to r because if this is the relation that must be satisfied?

Then there is a corresponding if you write this equation for r, then r must be equal to 1 over k times n pi + 1 pi by 2 - delta right. This is the location of the node on the radial r axis okay. That tells you exactly where on the radial distance, how far away from the center will the node occur. And this for the case when you have a potential which is not equal to 0 these nodes will occur at these values of r.

For the free electron these nodes occur at n pi + 1 pi by 2. So, this is the position of the nodes and notice that the nodes do not occur at the same distance. The nodes are either pulled or pushed depending on whether the phase shift delta is positive or negative. If the phase shift is push, if the phase shift is positive the position of the node will be pulled okay. That is what an attractive potential will do okay. See how the information about the potential is now coming okay.

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And if you have an attractive potential it will generate a positive phase shift and the node will be pulled in. So, this really depends on the phase shifts being positive or negative and if you have a attractive potential you have got a positive phase shift. If you have got a repulsive potential you have got a negative phase shift right.

Because that is going to determine whether the nodes are pulled or pushed. And if you look at the wave functions the radial functions themselves. (Refer Slide Time: 48:08)



Notice that in this case this is pushed in a repulsive potential in which you have a positive phase shift. It is pulled by an attractive phase shift when you have a negative potential okay. So this is how you get information about the target potential but of course much more detailed information is contained in that expression that we wrote earlier for tangent of delta in terms of that integral which is exact and if we can figure out how to deal with that how to develop approximations and so on.

We can get a lot of valuable information about the target potential from the phase shifts. So, that is what phase shift analysis is them out I will stop your for this class and continue from here in the next one.