

Select/Special Topics in ‘Theory of Atomic Collisions and Spectroscopy’
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Lecture 33
Lippman Schwinger Equation of potential scattering

Greetings, so welcome to the unit five of this course. This is again on Collisions. And I will call it as Part Two of Quantum Theory of Collisions because the first part we already have some 11 or 12 lectures in the Unit 1. And then, we took a detour and it is on second Quantization Random Phase Approximation, Feynman diagrams. So, we did that in Unit 2, 3 and 4. And now, we are resuming our discussion on Quantum Collisions.

So, in this unit, we will begin with the Lippman Schwinger Equation for Potential Scattering and subsequently we will also be doing the Coulomb scattering and then the resonances. So, this unit will basically have three classes: First on Lippman Schwinger equation, Second on Born approximations and third on Coulomb Scattering.
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In UNIT 5:

(1) Lippman-Schwinger equation of potential scattering.	L33
(2) Born approximations. Screened Coulomb scattering.	L34
(3) Coulomb Scattering.	L35

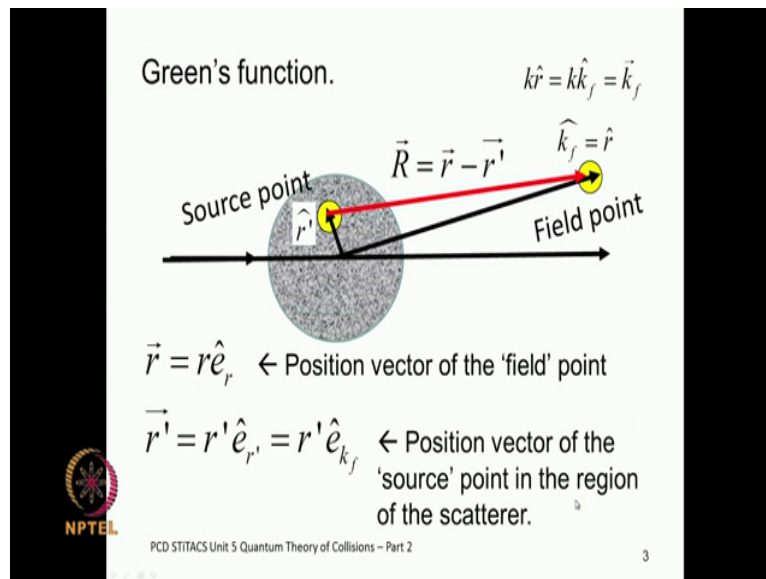
Units 6 (4 lectures) & 7 (4 lectures): Resonances

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And then, in subsequent units, we will have about eight classes on resonances. So, there will be four classes in unit 6 and another four in unit 7. So, there will be a total of eight classes on resonances.

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So, now, this is the picture of scattering that we have in front of us, that you have got a scattering target and then Incident beam which comes and interacts with it get scattered. And you can think of the scattering region as a certain spherical region of space. And different parts of the region would be responsible in some sort of a cause-effect relationship that, that would be the central cause for scattering seen at a given point.

So, you can think of this phenomenon in terms of a cause-effect relationship and we will introduce the Green's functions or the propagator to describe this. We have a different source point in the scattering region. And I will describe the field point with the position vector r , the source point with the position vector r' , with reference to the scattering center and the difference vector is $r - r'$.

So, this is the direction in which scattering is taking place with reference to the picture you have in this diagram.

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Reference: Joachain / Quantum Theory of Collisions / Chapter 5
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So, the essential equation, quantum mechanical equation that we are looking at, we are doing nonrelativistic quantum mechanics. And we have the Schrodinger equation with which we work. We can write it, in terms of the reduced potential, just to get rid of some constants like 2m and h cross square. So, we rewrite this equation, in terms of the potential. But essentially, it has got the same information as is available in the Schrodinger equation itself.

And you have on the right hand side of this equation, the inhomogeneous term and when you set it equal to 0, you get the corresponding homogeneous equation for 0 potential which is the problem for a free particle. So, this operator the del square + k square operator, this is known as the Helmholtz operator.

And we can have the Green's function for the free particle which is defined by this relation. So, this is, it defines the Green's function which is the solution for the Helmholtz operator. (Refer Slide Time: 03:51)



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We shall see that $\psi_{\vec{k}_i}(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \iiint d^3\vec{r}' G_0(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}(\vec{r}')$ is a solution of the Schrodinger equation. \uparrow Green's function is to be determined according to appropriate boundary conditions. "CATCH 22" ?

And now, we have to find out what would be the appropriate Green's function, which will describe the scattering process. So, this is a differential equation, but we can also cast it as an integral equation, okay. And what we propose is that, if we set up and a solution in this form, that the solution way of the Schrodinger equation which is this Ψ , that this can be expressed as a sum of the incident plain wave.


And an integral involving the Green's function and the potential, okay and then there is also a solution Ψ over here. And this is a little, this is some kind of cheating because what appears in the integrand is this wave function, which is what you really want to determine. So, you do not know it in the first place.

So, it is in some sense not really quite fair to put on the right hand side, what you have on the left hand side of the equation. But that is the formal structure of this relationship. And I will discuss this, the consequences about this. So, this is the Green's function. And this, we have to determine appropriately with due consideration to the boundary conditions, because the boundary conditions are essential to analyze the solutions.

You, when you have a differential equation; means you can get of very many different kinds of solutions will satisfy the differential equation. But the ones that we are interested in are, to be subjected to boundary conditions, which are appropriate to the physical problem that we are dealing with. So, this is a tricky situation. You have got a wave function on the right hand side in the integrand, which is actually the one on the left hand side.

And this is what one would regard as a Catch-22 situation that you are asking for the solution to be written in terms of what you really want to determine. And that problem is it falls into a vicious circle and you really cannot solve it. So, we will figure out how this is to be solved. But the first thing to do is that the formal structure of this equation is appropriate. That it does indeed describe the scattering process.

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$$\left[\frac{(-i\hbar\vec{\nabla})^2}{2m} + V(\vec{r}) \right] \psi(\vec{r}) = E\psi(\vec{r}) \quad \leftarrow \text{Schrodinger equation}$$

$$[\vec{\nabla}^2 + k^2]G_0(k, \vec{r}, \vec{r}') = \delta^3(\vec{r} - \vec{r}')$$

First, we show that

$$\psi_{\vec{k}_i}(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \iiint d^3\vec{r}' G_0(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}(\vec{r}')$$

is a solution of the Schrodinger equation


Method: operate on $\phi_{\vec{k}_i}(\vec{r}) + \iiint d^3\vec{r}' G_0(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}(\vec{r}')$
 by $[\vec{\nabla}^2 + k^2] \quad \leftarrow \text{Helmholtz operator}$

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And that is the first thing that we will consider. So, let us begin with what we have over here. So, we have the Schrodinger equation. The first thing we do is show that this is indeed a solution of the Schrodinger equation, although it is not a very useful solution because it is describing in the integrand, the wave function which is what you want to find.

So, it is not particularly useful. So, whether, whether or not it is useful is a different story. But that it is at least correct. But formally this is a solution of the Schrodinger equation, is something that we first test. And that can be seen by operating on the right hand side of this by the Helmholtz operator. So, as if you do that, you can very easily verify that in fact it is the solution.

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$$[\vec{\nabla}^2 + k^2] \psi_{\vec{k}_i}(\vec{r}) =$$

$$= [\vec{\nabla}^2 + k^2] \left\{ \phi_{\vec{k}_i}(\vec{r}) + \iiint d^3\vec{r}' G_0(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}(\vec{r}') \right\}$$

$[\vec{\nabla}^2 + k^2] \phi_{\vec{k}_i}(\vec{r}) = 0 \quad \leftarrow \text{Homogeneous equation 'free' particle}$

$$= \iiint d^3\vec{r}' [\vec{\nabla}^2 + k^2] G_0(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}(\vec{r}')$$

$$[\vec{\nabla}^2 + k^2] G_0(k, \vec{r}, \vec{r}') = \delta^3(\vec{r} - \vec{r}')$$

$$= \iiint d^3\vec{r}' \delta^3(\vec{r} - \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}(\vec{r}')$$

$[\vec{\nabla}^2 + k^2] \psi_{\vec{k}_i}(\vec{r}) = U(\vec{r}) \psi_{\vec{k}_i}(\vec{r})$

Schrodinger equation

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So, let us do that as the first step. So, you operate on this formal structure, formal solution that has been proposed by the Helmholtz operator. And now, you know that, this is the

homogeneous equation for a free particle when the potential is zero. So, the first term gives you nothing, it gives you zero.

And then, you have the Helmholtz operator operating over here. So, now you know that you are going to pick up a delta function from this operation; because that is how the Green's function is defined, right. So, del square + k square operating on the Green's function gives you the delta function.

So, this is the Dirac delta. So, you get a Dirac delta from this operation. And then, you are going to integrate this potential on this wave function multiplied by the Dirac delta. So, you will end up having a Dirac delta integration. So, here you have the Dirac delta inserted in place of del square plus k square, operating on the Green's function.

And you find that when you carry out this delta function integration, you recover the Schrodinger equation. So, we know that, okay, whatever we proposed as an integral equation is formally correct, regardless of the fact that, it is not particularly useful at this stage. But then, we will figure out how to develop some sort of an approximation to it so that it will become useful, okay.

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$$\psi_{\vec{k}_i}(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \iiint d^3\vec{r}' G_0(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}(\vec{r}')$$

↑ Lippman-Schwinger ↑
 equation for potential scattering.

↑ Green's function is to be determined according to appropriate boundary conditions.

Determination of the Green's function: $G_0(k, \vec{r}, \vec{r}')$

Take the Fourier transform of $G_0(k, \vec{r}, \vec{r}')$

$$G_0(k, \vec{R}) = \frac{1}{(2\pi)^3} \iiint d^3\vec{k}' g(\vec{k}') e^{i\vec{k}' \cdot \vec{R}}$$

Omit $k \updownarrow$

$$i.e. G_0(\vec{R}) = \frac{1}{(2\pi)^3} \iiint d^3\vec{k}' g(\vec{k}') e^{i\vec{k}' \cdot \vec{R}}$$

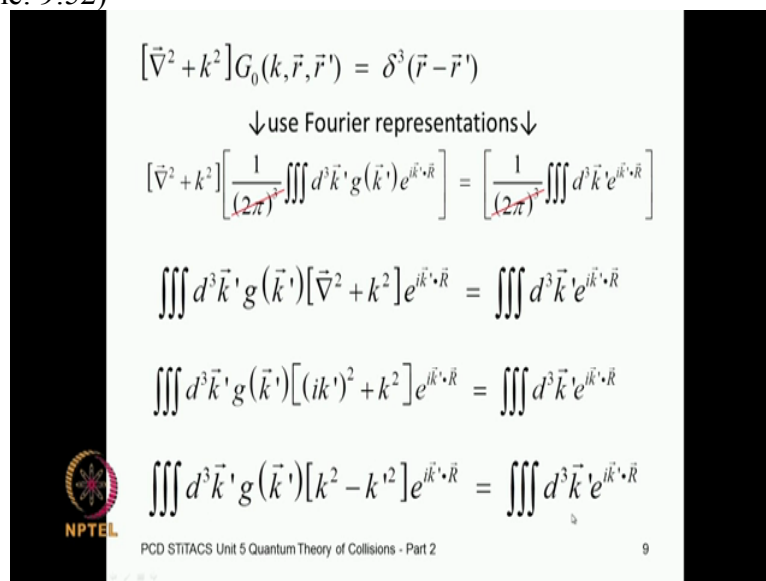
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So, this is the Green's function. But we do not know what the Green's function is. And this Green's function will have to be chosen according to appropriate boundary conditions; because just like the differential equation requires appropriate boundary conditions to be solved, the integral equation requires the Green's function to be defined with reference to appropriate boundary conditions.

And we know that in Collision Physics, we make use of these outgoing wave boundary conditions. So, you remember that. And we will put those boundary conditions to describe the Green's function in the Collision process. So, first we have to determine the Green's function G_0 with reference to appropriate boundary conditions.

So, what we will do is take the Fourier transform of the Green's function. So, let us define this Fourier transform. And just to simplify the notation I will drop this case. So, instead of $G_0(k, \vec{r}, \vec{r}')$, I will write this only as $G_0(\vec{r})$. So, this is nothing but the Fourier representation of the Green's function. This is the usual standard for your representation of the Green's function.

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$$[\nabla^2 + k^2]G_0(k, \vec{r}, \vec{r}') = \delta^3(\vec{r} - \vec{r}')$$

↓ use Fourier representations ↓

$$[\nabla^2 + k^2] \left[\frac{1}{(2\pi)^3} \iiint d^3\vec{k}' g(\vec{k}') e^{i\vec{k}' \cdot \vec{R}} \right] = \left[\frac{1}{(2\pi)^3} \iiint d^3\vec{k}' e^{i\vec{k}' \cdot \vec{R}} \right]$$

$$\iiint d^3\vec{k}' g(\vec{k}') [\nabla^2 + k^2] e^{i\vec{k}' \cdot \vec{R}} = \iiint d^3\vec{k}' e^{i\vec{k}' \cdot \vec{R}}$$

$$\iiint d^3\vec{k}' g(\vec{k}') [(i\vec{k}')^2 + k^2] e^{i\vec{k}' \cdot \vec{R}} = \iiint d^3\vec{k}' e^{i\vec{k}' \cdot \vec{R}}$$

$$\iiint d^3\vec{k}' g(\vec{k}') [k^2 - k'^2] e^{i\vec{k}' \cdot \vec{R}} = \iiint d^3\vec{k}' e^{i\vec{k}' \cdot \vec{R}}$$

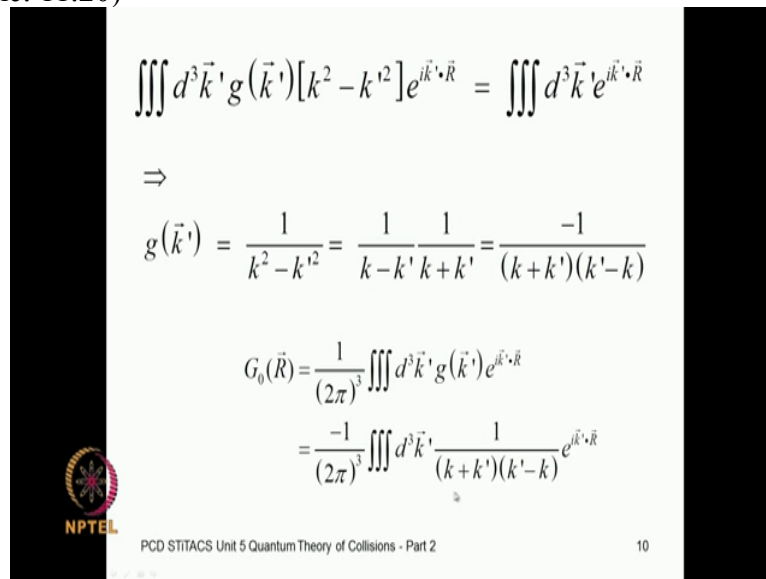
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And we will also have the usual Fourier representation of the right hand side of this which is the Fourier representation of the delta function. So, which is a sum of these exponential terms, right? So, when you sum up all these exponential terms integrate over the whole volume in the k space, you get the corresponding Fourier representation of the Dirac Delta.

So, instead of G_0 and delta on this side, we use the corresponding Fourier representations. So, here they are. So, now, you have got this integral of, in the momentum space or the k space. And then, you have got these coefficients $g(\vec{k}')$. And now you have $\nabla^2 + k^2$ operating on $e^{i\vec{k}' \cdot \vec{R}}$ which you can see, immediately will give you this $i\vec{k}'^2$ from the ∇^2 term.

This will come as a k^2 multiplier. Right-hand side is pretty much the same. The $(2\pi)^3$ on both sides of the equations have cancelled each other, ok. So, we are getting a pretty straightforward relationship now. And now, you can see that you have in the integrand, both

sides of the integrations, are integrations in the k space. And the integrand has got one factor which is common e to the i k prime dot R on both sides.
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Slide 10 content:

$$\iiint d^3\vec{k}' g(\vec{k}') [k^2 - k'^2] e^{i\vec{k}' \cdot \vec{R}} = \iiint d^3\vec{k}' e^{i\vec{k}' \cdot \vec{R}}$$

$$\Rightarrow g(\vec{k}') = \frac{1}{k^2 - k'^2} = \frac{1}{k - k'} \frac{1}{k + k'} = \frac{-1}{(k + k')(k' - k)}$$

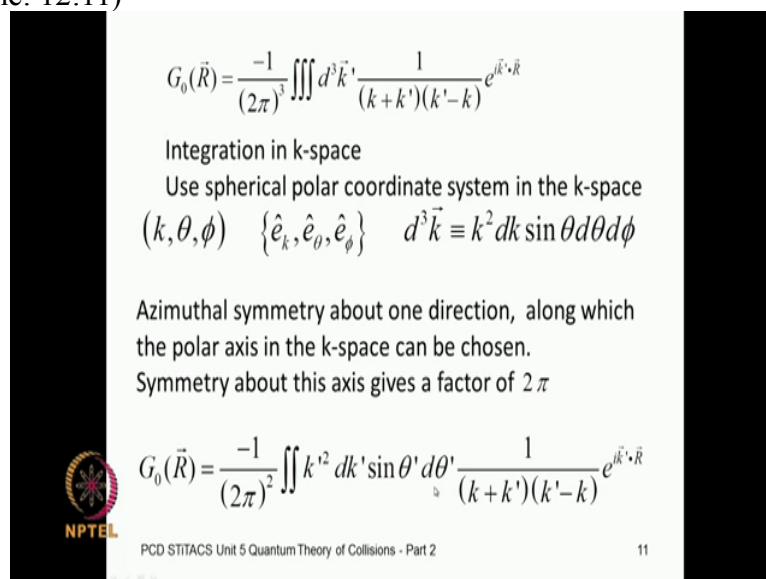
$$G_0(\vec{R}) = \frac{1}{(2\pi)^3} \iiint d^3\vec{k}' g(\vec{k}') e^{i\vec{k}' \cdot \vec{R}}$$

$$= \frac{-1}{(2\pi)^3} \iiint d^3\vec{k}' \frac{1}{(k + k')(k' - k)} e^{i\vec{k}' \cdot \vec{R}}$$

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So, if you look at this, the, this is the definite integral in the k space over the entire k space. So, the corresponding integrands will have to be the same and that tells us that this gk prime must be the inverse of k square - k prime square, so that the product will give you the unity, which you have on the right hand side, okay.

So, this is what you get for the Fourier transform. And here you can factor this into k + k prime and k prime - k. And you recognize that the Green's function is now given by this integral. So, this is mathematically completely equivalent to what we started out with using the Fourier transforms, okay.
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Slide 11 content:

$$G_0(\vec{R}) = \frac{-1}{(2\pi)^3} \iiint d^3\vec{k}' \frac{1}{(k + k')(k' - k)} e^{i\vec{k}' \cdot \vec{R}}$$

Integration in k-space
Use spherical polar coordinate system in the k-space
 $(k, \theta, \phi) \quad \{\hat{e}_k, \hat{e}_\theta, \hat{e}_\phi\} \quad d^3\vec{k} \equiv k^2 dk \sin\theta d\theta d\phi$

Azimuthal symmetry about one direction, along which the polar axis in the k-space can be chosen.
Symmetry about this axis gives a factor of 2π

$$G_0(\vec{R}) = \frac{-1}{(2\pi)^2} \iint k'^2 dk' \sin\theta' d\theta' \frac{1}{(k + k')(k' - k)} e^{i\vec{k}' \cdot \vec{R}}$$

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Now, having got this, notice that what you are integrating out, there is a certain symmetry that you can exploit, because in this symmetry, you can, you have the volume element in the

k space which is given as $k^2 dk \sin \theta d\theta d\Phi$. So, this is the spherical polar coordinates in the reciprocal space in the k space.

And if you exploit the azimuthal symmetry about one direction about which you can choose the polar axis then integration of the azimuthal angle about that will give you a factor of 2π . So, let us get that out of our way and the rest of the integration is now only over two degrees of freedom which is θ and Φ .

So, you have got the $k^2 dk \sin \theta d\theta$, right. The integration variables I am using as the prime because that is what we started out with. So, these are the prime variables k' , k'^2 , dk' , $\sin \theta'$, $d\theta'$. This is the integrand $1/(k+k')(k'-k)$, $e^{i\vec{k}' \cdot \vec{R}}$, okay. (Refer Slide Time: 13:26)

$$G_0(\vec{R}) = \frac{-1}{(2\pi)^2} \iiint k'^2 dk' \sin \theta' d\theta' \frac{1}{(k+k')(k'-k)} e^{i\vec{k}' \cdot \vec{R}}$$

$$G_0(\vec{R}) = \frac{-1}{(2\pi)^2} \int_{k'=0}^{\infty} \frac{k'^2}{(k+k')(k'-k)} dk' \int_{\theta'=0}^{\pi} \sin \theta' d\theta' e^{ik'R \cos \theta'}$$


$$d(\cos \theta') = -\sin \theta' d\theta'$$

$$G_0(\vec{R}) = \frac{-1}{(2\pi)^2} \int_{k'=0}^{\infty} \frac{k'^2}{(k+k')(k'-k)} dk' \int_{\cos \theta'=-1}^{\cos \theta'=1} d(\cos \theta') e^{ik'R(\cos \theta')}$$

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Now look at the integrand over here. So, now we can separate out the integration over θ and k these are independent degrees of freedom. So, what you are integrating over θ actually θ' . So, the range of θ' is from 0 to π range of Φ' was from 0 to 2π which is what gave us the factor of 2π . So, now you have separated the integration over θ' and π .

And it is convenient as we do in so many problems right from high school mathematics to change the integration variable to $\cos \theta'$. And then write this integration appropriately, you have to put the limits instead of the limits for θ' . You now put the limits for $\cos \theta'$ but mind you there is a minus sign here. So, the limits go from $\cos \theta'$ equal to -1 to $= 1$, okay. (Refer Slide Time: 14:20)



$$G_0(\vec{R}) = \frac{-1}{(2\pi)^2} \int_{k'=0}^{\infty} \frac{k'^2}{(k+k')(k'-k)} dk' \int_{\cos\theta'=-1}^{\cos\theta'=1} d(\cos\theta') e^{ik'R(\cos\theta')}$$

$$G_0(\vec{R}) = \frac{-1}{(2\pi)^2} \int_{k'=0}^{\infty} \frac{k'^2}{(k+k')(k'-k)} dk' \left[\frac{e^{ik'R(\cos\theta')}}{ik'R} \right]_{\cos\theta'=-1}^{\cos\theta'=1}$$


$$G_0(\vec{R}) = \frac{-1}{(2\pi)^2} \int_{k'=0}^{\infty} \frac{k'}{(k+k')(k'-k)} \frac{e^{ik'R} - e^{-ik'R}}{iR} dk'$$

$$G_0(\vec{R}) = \frac{-1}{(2\pi)^2} \int_{k'=0}^{\infty} \frac{k'}{(k+k')(k'-k)} \frac{2\sin(k'R)}{R} dk'$$

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So, this is pretty straightforward as such. So, this is the integral over the polar angle theta prime, okay. So, carry out this integration you have got e to the ik prime r cos theta prime over ik prime R. And then, you have to take the difference of cos theta over the upper limit less the lower limit, okay.

So, let us do that. So, this is the difference at the two limits. You have got the denominator ik prime R, right. So, now what do you have? You have e to the ik prime R - e to the - ik prime R. And you can write this as a sinusoidal function. And then, get rid of the common terms 2i and so on. So, that is straightforward algebra and this is the expression that you get. (Refer Slide Time: 15:25)



$$G_0(\vec{R}) = \frac{-1}{2\pi^2 R} \int_{k'=0}^{\infty} \frac{k' \sin(k'R)}{(k'+k)(k'-k)} dk'$$

The integrand is an even function of k'

Extend the range of integration to $k' < 0$
(non-physical; but mathematically admissible)
so that we can use contour integration to
circumvent the 'poles' at $k'=+k$ and at $k'=-k$.

$$G_0(\vec{R}) = \frac{-1}{2\pi^2 R} \frac{1}{2} \int_{k'=-\infty}^{\infty} \frac{k' \sin(k'R)}{(k'+k)(k'-k)} dk'$$

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Now, let us take this to the top of the next slide. And if you look at the integrand, the integral is an even function of k prime. So, you can extend the integration from k prime = 0 to infinity 2k prime = - infinity to + infinity and then take half of it. So, mathematically it is absolutely

satisfactory; physically it is meaningless because in the spherical polar coordinate system you have the space covered by the polar angle going from 0 to pi.

The azimuthal angle going from 0 to 2pi and the third degree of freedom going from 0 to infinity in the reciprocal space it is the k or the k prime, okay. So, physically k prime having negative values is of absolute no significance but mathematically our interest over here is to determine what is the value of this integral.

And we can use complex analysis to evaluate this integral by exploiting the fact that, okay you have got an integral, in which, you are having an even function. So, so, you extend the range of integration which is from k prime = 0 to infinity. You extend it to negative values of k prime and let it go from minus infinity to plus infinity. And then, use contour integration to deal with the poles.

You see that there are there would be poles at k prime = + k and k prime = - k. So, then, you can use contour integration to handle those poles, okay. So, here you are, so, now because you have extended the range of integration which was from 0 to infinity. You now have the range of integration from minus infinity to plus infinity. You have picked a factor of half so that mathematically you have exactly the same value for the net integration, okay. (Refer Slide Time: 17:22)



$$G_0(\vec{R}) = \frac{-1}{2\pi^2 R} \frac{1}{2} \int_{k'=-\infty}^{\infty} \frac{k' \sin(k'R)}{(k'+k)(k'-k)} dk'$$

$$G_0(\vec{R}) = \frac{-1}{2\pi^2 R} \frac{1}{2} \int_{k'=-\infty}^{\infty} \left[\frac{1}{2} \left\{ \frac{1}{(k'+k)} + \frac{1}{(k'-k)} \right\} \right] \frac{e^{ik'R} - e^{-ik'R}}{2i} dk'$$

$$G_0(\vec{R}) = \left[\begin{aligned} &\frac{-1}{16\pi^2 Ri} \int_{k'=-\infty}^{\infty} e^{ik'R} \left\{ \frac{1}{(k'+k)} + \frac{1}{(k'-k)} \right\} dk' + \\ &+ \frac{(+1)}{16\pi^2 Ri} \int_{k'=-\infty}^{\infty} e^{-ik'R} \left\{ \frac{1}{(k'+k)} + \frac{1}{(k'-k)} \right\} dk' \end{aligned} \right]$$

Two integrals

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So, this is the integral that you now have to determine which is from minus infinity to plus infinity. And we once again express this sine function in how we had seen it earlier in terms of e to the ik prime R - e to the ik prime R divided by 2i, okay. We had put it in the sinusoidal form, just to make the even nature of the integral explicitly manifest. So, now we go back to this form and we now write it as 2 integrals.

One coming from this term and the other coming from this term, so, there are now two integrals to evaluate, okay. So, the first one is coming from e to the ik prime R and the other is coming from this second term e to the - ik prime R. And then, of course, you have this factor which is common to both, right. So, these are the two integrals which we now have to determine.

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$$G_0(\vec{R}) = \frac{-1}{16\pi^2 Ri} I_1 + \frac{1}{16\pi^2 Ri} I_2$$

$$I_1 = \int_{k'=-\infty}^{\infty} e^{ik'R} \left\{ \frac{1}{(k'+k)} + \frac{1}{(k'-k)} \right\} dk'$$

$$I_2 = \int_{k'=-\infty}^{\infty} e^{-ik'R} \left\{ \frac{1}{(k'+k)} + \frac{1}{(k'-k)} \right\} dk'$$

Both I_1 and I_2 have SIMPLE POLES
 at $k' = +k$
 and at $k' = -k$
 in the complex k' -plane

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And these two integrals I have represented over here as I1 and I2. So, these are the two integrals that we have to determine. What we have to keep in mind is that these are to be evaluated appropriately with reference to the boundary conditions, which must be referred to without which the solution has got no meaning okay.

So, here we are, so we have got the two integrals to be determined I1 and I2. We have to be careful while evaluating these integrals because both of them have got poles. And these poles are at k prime = + k and k prime = - k.

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Cauchy's Residue Theorem

$$f(z) = \sum_{n=-\infty}^{+\infty} a_n (z - z_0)^n \quad \text{Laurent expansion}$$

contour C encircles one isolated singularity at z_0

$$\frac{1}{2\pi i} \oint_C f(z) dz = a_{-1}, \text{ coefficient of } \left(\frac{1}{z - z_0} \right)$$

a_{-1} is the residue of $f(z)$ at $z = z_0$

$a_{-1} \leftrightarrow \frac{1}{z - z_0}$

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So, we will make use of contour integration and use the Cauchy's residue theorem which you are all familiar with. So, this is just that if you have a large expansion, of a function of a complex variable, then, this integral over here, over a closed loop, will be given by the residue, which is just this factor 1 over $z - z_0$ of in this Laurent series expansion. (Refer Slide Time: 19:38)

Jordan's lemma

If the only singularities of $f(z)$ are isolated poles,

$$\lim_{R \rightarrow \infty} \oint e^{iaz} f(z) dz = 0$$

Note!

$a > 0$

and

$\lim_{R \rightarrow \infty} |f(z)| \rightarrow 0$

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So that is theorem of residues and in particular, we will use a Jordan's lemma, because we have got in the integration one factor which goes as e to the iaz . We have already seen that; so, having seen that, it would be obvious to you that appropriately we must use the Jordan's lemma which tells us that if the only singularities of the function are isolated poles, then you can evaluate this integral according to this relation.

So, it is basically just a straightforward extension of the Cauchy's residue theorem. So, we will make use of the Jordan's lemma and notice that the Jordan lemma requires this coefficient a to be a positive. And we have to be careful about it because if it is not positive,

then the contour has to be closed in the lower half of the plane rather than the upper half of the plane. So that is the only thing that we are going to have to keep track on. (Refer Slide Time: 20:34)

$$I_1 = \int_{k'=-\infty}^{\infty} e^{ik'R} \left\{ \frac{1}{(k'+k)} + \frac{1}{(k'-k)} \right\} dk'$$

integrand: $f(k') = e^{ik'R} \left\{ \frac{1}{(k'+k)} + \frac{1}{(k'-k)} \right\}$

residue of $f(k')$ at $k' = k$ is e^{ikR}

residue of $f(k')$ at $k' = -k$ is e^{-ikR}

$I_{C_1} = 0$

Jordan's lemma

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So, in this case, we have two integrals. So, let us look in the first integral and in the first integral, this k prime is to be integrated from minus infinity to plus infinity, right. And the residue of $f(k')$ at k' prime, equal to k is, e^{ikR} , as you can see. So, this is the residue at k' prime = $-k$, it will be $-ikR$. So, depending on this, we have to close the contour appropriately, okay.

So let us have a look at what result we get from the Jordan's lemma. And that will of course depend on how we choose the contour itself. So, we can choose the contour by hopping over these two poles, okay. And in this case, you can immediately see that this integral will vanish, okay.

So, this will vanish if you choose this contour to hop over these two poles. You can, of course, choose other possible contours by including these two poles or including one at a time or both at a time and depending on what you do and how you choose this contour you will obviously get a different answer.

(Refer Slide Time: 21:54)

$$I_1 = \int_{k'=-\infty}^{\infty} e^{ik'R} \left\{ \frac{1}{(k'+k)} + \frac{1}{(k'-k)} \right\} dk'$$

$$I_1^{C_1} = 0$$

$e^{-i\omega t}$

$$I_1^{C_2} = 2\pi i [e^{ikR} + e^{-ikR}]$$

Outgoing *plus* Ingoing wave
time-dependence:

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So, here was our first choice of the contour, when you hopped over both the poles. And the solution for this integral is 0. Now, if you now include both the poles, then, the solution will be e to the ikR and e to the $-ikR$. And what is, what are these functions? Now, this is only the solution of the space part of the Schrodinger wave function. There is also a time dependence, right.

For the stationary says the time dependence is given by e to the $-i\omega t$. And when you multiply this by e to the $-i\omega t$, this e to the solution will become e to the $ikR - \omega t$ for this term and e to the $-kR + \omega t$. So, this will become a spherical outgoing wave and this will become a spherical in going wave right. So, you will get a solution in this case which is a superposition of an outgoing wave plus an in going wave.

What kind of a solution are we looking for? In Collisions, we are looking for outgoing wave solutions. So, the first contour did not give us what we wanted. It gave us 0; the second contour also does not give us a solution that we wanted. It does give us an outgoing way but it does not give us only an outgoing wave. It gives us an outgoing wave and also an in going wave. So, that is also not the one that we are looking for.
(Refer Slide Time: 23:24)

$$I_1 = \int_{k'=-\infty}^{\infty} e^{ik'R} \left\{ \frac{1}{(k'+k)} + \frac{1}{(k'-k)} \right\} dk'$$

$$I_1^{C_3} = 2\pi i e^{-ikR}$$

Ingoing wave

$k' = -k \uparrow \quad \uparrow k' = +k$

time-dependence:
 $e^{-i\omega t}$

$$I_1^{C_4} = 2\pi i e^{+ikR}$$

Outgoing wave

$k' = -k \uparrow \quad \uparrow k' = +k$

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How about this, this contour if you include the pole at $-k$, but exclude the pole at $+k$, then, you get e^{-ikR} , which is again an ingoing wave. So, that is not what we want. So, now if you exclude the pole at $-k$ and include the one at $+k$, then, you get an outgoing wave solution.

And that is the one that we are looking for as a solution to our scattering problem. So, it is just a matter of choosing the appropriate contour. So, what the Jordan's lemma tells you is, how to evaluate the integral in this particular case. But then, it is up to you to use the appropriate boundary condition.

And that is always the case, whether it is you are solving a differential equation for scattering or you are solving an integral equation for scattering; because in both, you know, these are only mathematically inverses of each other. But both require the boundary conditions to be referred to one way or another, okay.
 (Refer Slide Time: 24:30)

$$G_0(\vec{R}) = \frac{-1}{16\pi^2 Ri} I_1 + \frac{1}{16\pi^2 Ri} I_2$$

$$I_1 = \int_{k'=-\infty}^{\infty} e^{ik'R} \left\{ \frac{1}{(k'+k)} + \frac{1}{(k'-k)} \right\} dk'$$

$$I_2 = \int_{k'=-\infty}^{\infty} e^{-ik'R} \left\{ \frac{1}{(k'+k)} + \frac{1}{(k'-k)} \right\} dk'$$

Evaluation of I_2

The integrand has \downarrow Hence, the contour must be closed in the LOWER half of the complex k' plane.

Remember Jordan's lemma?

$e^{-ik'R}$

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So, this is now the solution in for the first integral, okay. In the second integral, you do not have e to the ik prime R , but you have got to the $-ik$ prime R , okay. So, you have to be a little careful in evaluating the Jordan's lemma. And what you will have to do in this case is to close the contour in the lower half of the complex plane. So let us do that.
(Refer Slide Time: 24:59)

$$I_2 = \int_{k'=-\infty}^{\infty} e^{-ik'R} \left\{ \frac{1}{(k'+k)} + \frac{1}{(k'-k)} \right\} dk'$$

Outgoing plus Ingoing wave

$$I_2^{C_1} = -2\pi i [e^{ikR} + e^{-ikR}]$$

↑ minus sign as the path is clockwise

time-dependence:

$$e^{-i\omega t}$$

$$I_2^{C_2} = 0$$

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So, now we close on the lower half of the complex plane to evaluate the integral I_2 . And now I will go through this little quickly because we know how these contours are being evaluated, say, if you take this contour C_1 , in which, you include both the poles. But then, close the contour on the lower half, then, you get a sum of outgoing wave plus an in going wave.

When you consider the time dependence, mind you that, unless you plug in the time dependence, the terms outgoing and in going have got absolutely no significance because the time parameter has to be there. That is the one which is telling you whether a surface of constant phase is a spherical surface which is moving out of the center or it is converging on to the center, okay.

So, that has to be done because it, it is a travelling wave. And you have to refer to it, with reference to, the time parameter. So, make sure that you insert the time dependence e to the $-i\omega t$ at least in your mind so that you know what talking about and why this is an outgoing wave and why it is an in going wave.

So, you get a combination of outgoing and in going wave on this contour C_1 . Contour C_2 hops over both the poles and you get zero, okay because it hops over both the poles. So, on the contour C_2 , you the value of I_2 is 0.
(Refer Slide Time: 26:34)

$$I_2 = \int_{\epsilon-i\infty}^{\infty} e^{-ikR} \left\{ \frac{1}{(k'+k)} + \frac{1}{(k'-k)} \right\} dk'$$

Outgoing wave

$$I_2^{C_3} = -2\pi i e^{+ikR}$$

time-dependence:

$$e^{-i\omega t}$$

Ingoing wave

$$I_2^{C_4} = -2\pi i e^{-ikR}$$

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And then, you have two other possibilities: one is to hop over this, but include this and the other is to include this but hop over this. So, you have got two other Contour C3 and C4 and you find that it is the contour C3, which gives you the outgoing wave e^{+ikR} . So that will be the right contour to be chosen. And the Green's function will be defined with reference to this particular contour, okay.
(Refer Slide Time: 27:02)

$$G_0(\vec{R}) = \frac{-1}{16\pi^2 Ri} I_1 + \frac{1}{16\pi^2 Ri} I_2$$

$$G_0^+(\vec{R}) = \frac{-1}{16\pi^2 Ri} I_1^{outgoing} + \frac{1}{16\pi^2 Ri} I_2^{outgoing}$$

$$G_0^+(\vec{R}) = \frac{-1}{16\pi^2 Ri} I_1^{C_4} + \frac{1}{16\pi^2 Ri} I_2^{C_3}$$

$$G_0^+(\vec{R}) = \frac{-1}{16\pi^2 Ri} [2\pi i e^{+ikR}] + \frac{1}{16\pi^2 Ri} [-2\pi i e^{+ikR}]$$

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So, you have these two integrals that we wanted to determine. And we now know how to evaluate those with reference to the outgoing wave boundary conditions. Both of these integrals I1 and I2 are to be evaluated with reference to that. And since we are focusing attention on the outgoing wave boundary condition, I put a superscript plus to remind me that this is the Green's function appropriate for the outgoing wave boundary condition okay.

So, this is indicated by the superscript plus on the Green's function. So, the contour appropriate for I1 was the contour which I had called as C4 and the contour appropriate for I2

which gave us outgoing solution is what we had called as C3. So, that is just a matter of simple notation in our context. And these are the solutions you have to sum up these two terms, okay.

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$$G_0^+(\vec{R}) = \frac{-1}{16\pi^2 Ri} [2\pi i e^{ikR}] + \frac{1}{16\pi^2 Ri} [-2\pi i e^{ikR}]$$

$$G_0^+(\vec{R}) = \frac{-e^{ikR}}{4\pi R}$$
Outgoing boundary conditions incorporated

$$\psi_{\vec{k}_i}^-(\vec{r}) = \phi_{\vec{k}_i}^-(\vec{r}) + \iiint d^3\vec{r}' G_0(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^-(\vec{r}')$$

↑ Lippman-Schwinger ↑
 equation for potential scattering.

↑ Green's function is to be determined according to appropriate boundary conditions.

$$\psi_{\vec{k}_i}^+(\vec{r}) = \phi_{\vec{k}_i}^+(\vec{r}) + \iiint d^3\vec{r}' G_0^+(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^+(\vec{r}')$$

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So, let us go ahead and carry out this summation and the common terms you have got a factor of 2 pi here, you have got 16 pi square here, you have got 1 over R in both the terms. So, you put all the terms together simplify and essentially it adds up to -e to the ikR by R divided by 4 PI, okay. So, that is the Green's function with outgoing wave boundary condition properly incorporated.

So, okay, now, we have got the Green's function with the outgoing wave boundary condition. This goes into the Lippman-Schwinger equation. So, we have got the formal solution now. So, everything is what is how we wanted it except for the two things which we still have to address. One as to what we are going to do about the fact that the integrand has got, what is there on the left-hand side.

And we do not know it. So, you are giving the solution in terms of the problem okay. So that is cheating. So, we are going to have to address that. We will. And the other thing we have to remember is that the reason we are doing Mathematics or physics or Quantum Mechanics is because we are, you know, you are doing an experiment, okay.

We as physicists we want the mathematical theory to simulate the experiment appropriately so that it describes the experiment. It gets you; it helps you get the solutions. And when you carry out your measurements, because measurement is fundamental to physics and when you carry out measurements, you keep a detector somewhere.

And then, in this detector from the observations, in this detector how do you interpret the results and get information about the target. So, that is the whole reason why you are doing Quantum Mechanics. It is not just because you want to solve a Differential equation or an Integral equation but because you want to do some physics.

And what is the physics over here? That there is a detector, which is, where is the detector? It is very far. It is in the asymptotic region. It is in the region for all practical purposes as R tends to infinity. So, we are really not interested in the solution as it is. But we are interested in the asymptotic solution. So, that is the second thing we have to put in. One is to figure out how to address this function second to get the asymptotic form.

And just to remind us that we are using the outgoing wave boundary conditions. I will always keep a superscript plus on the Green's function and also on the wave function you know this is very important because when you do photo ionization you have to make use of the ingoing wave boundary conditions but in this case we make use of the outgoing wave boundary conditions

(Refer Slide Time: 31:00)

The poles are at $k' = \pm k$

Displace the poles to $k' = \pm(k + i\varepsilon')$

and take the limit $\varepsilon' \rightarrow 0^+$

$$k'^2 = (k^2 + i2k\varepsilon' + \varepsilon'^2)$$

$$k'^2 \approx (k^2 + i\varepsilon); \quad \varepsilon = 2k\varepsilon'$$

$$G_0^+(\vec{R}) = \frac{-1}{(2\pi)^3} \lim_{\varepsilon' \rightarrow 0^+} \iiint d^3\vec{k}' \frac{e^{i\vec{k}' \cdot \vec{R}}}{k'^2 - k^2 - i\varepsilon}$$

The path of integration is now along the real k' axis, apart from the semi-circle at infinity

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You can also carry out the integration by displacing the pole slightly. And this is just a tiny mathematical detour which may be of interest to you and depending on what book you are referring to, you will find solutions which look very similar. But what they do is they; they displace these poles by an infinitesimal amount and then carry out the integration entirely along the real axis rather than hopping over the pole.

So, mathematically it is a completely equivalent process and then you can take the limit if you have displaced it through this epsilon prime. So, you add this I epsilon prime or subtract it, okay. Then, you have to take the limit as epsilon prime goes to 0 and then carry out the

integration. So, essentially, you get the same result. So, it will not give you any fundamentally new thing.
 (Refer Slide Time: 31:57)

$$\psi_{\vec{k}_i}^+(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \iiint d^3\vec{r}' G_0^+(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^+(\vec{r}')$$

Evaluation of this → integral

$$\uparrow G_0^+(\vec{R}) = \frac{-e^{ikR}}{4\pi R}$$

$$J = -\frac{1}{4\pi} \iiint d^3\vec{r}' \frac{e^{-ikR}}{R} U(\vec{r}') \psi_{\vec{k}_i}^+(\vec{r}')$$

Our interest: asymptotic limit $r \rightarrow \infty$

$$R = |\vec{r} - \vec{r}'|$$

$$= \left[(\vec{r} - \vec{r}') \cdot (\vec{r} - \vec{r}') \right]^{\frac{1}{2}} \quad R = r \left[1 + \frac{r'^2 - 2\vec{r} \cdot \vec{r}'}{r^2} \right]^{\frac{1}{2}}$$

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So, now we are interested in the evaluation of this integral. And this integral is what I have represented by the letter J, ok. This we already know. This integral, this overall integral is J, the Green's function with outgoing wave boundary condition is minus of e to the ik R by 4 PI R. So, the 4 pi is here and the R is here. And we will now seek the limit R tending to infinity, okay.

Now, you remember what this capital R was. In the picture of scattering, which I showed you, I had a field point which was r and a source point which was r prime. Capital R is the difference r - r prime, okay.
 (Refer Slide Time: 32:53)

$$\psi_{\vec{k}_i}^+(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \iiint d^3\vec{r}' G_0^+(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^+(\vec{r}')$$

Evaluation of this → integral

$$\uparrow G_0^+(\vec{R}) = \frac{-e^{ikR}}{4\pi R}$$

$$J = -\frac{1}{4\pi} \iiint d^3\vec{r}' \frac{e^{-ikR}}{R} U(\vec{r}') \psi_{\vec{k}_i}^+(\vec{r}')$$

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$$R = |\vec{r} - \vec{r}'|$$

$$= \left[(\vec{r} - \vec{r}') \cdot (\vec{r} - \vec{r}') \right]^{\frac{1}{2}} \quad R = r \left[1 + \frac{r'^2 - 2\vec{r} \cdot \vec{r}'}{r^2} \right]^{\frac{1}{2}}$$

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So, it will tell you, how things take place at the field point because there is a cause for it, there is a reason for it. And what is the reason that there is a scatterer. And where is the

Scatterer? It is at the source point which is spread out. It is not centered focused at a given point but it is in the entire scattering region.

So, it is located at r' . So, this is capital R which is the distance between r and r' , the difference between the field point and the source point which is just the square root of the inner product of $r - r'$ with itself. And you can expand this, this factor to the power one-half, okay. You can carry out an expansion and then develop an approximation as r tends to infinity because that is a region of interest okay.

(Refer Slide Time: 33:50)

Source point $\vec{R} = \vec{r} - \vec{r}'$ Field point

$$R = r \left[1 + \frac{r'^2 - 2\vec{r} \cdot \vec{r}'}{r^2} \right]^{\frac{1}{2}}$$

$$R = r \left[1 + \frac{1}{2} \frac{r'^2 - 2rr' \cos \theta}{r^2} + \frac{1}{1 \times 2} \left(\frac{1}{2} - 1 \right) \frac{(r'^2 - 2rr' \cos \theta)^2}{r^4} - \dots \right]$$

$$R = r \left[1 + \frac{1}{2} \frac{r'^2 - 2rr' \cos \theta}{r^2} + \frac{1}{1 \times 2} \frac{\left(\frac{1}{2} - 1 \right) (r'^4 - 4rr'^3 \cos \theta + 4r^2 r'^2 \cos^2 \theta)}{r^4} + \dots \right]$$

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So, this expansion, so, this is the picture that we have. So this is $r - r'$. This is the same picture that I showed you earlier. And I will not discuss these steps in between. You know how to do that. You would have done that number of times by when you dealt with multiple expansions, for example, r and so on.

So, there are large number of problems in mathematical physics, electrodynamics and quantum mechanics where you make exactly the same kind of power series expansion and develop an approximation so I will not discuss this in detail I do have most of the intermediate steps on the slides.

So, you can always refer to the PDF and then take it from there if you need to. But you won't have to I am pretty sure about it. So, these are blue arrows on the side. They remind me that I can skip this part of the discussion, okay. And they will also remind you that I am going to skip the next slide, okay for exactly the same reason, okay.

(Refer Slide Time: 34:50)

$$R = r \left[1 + \frac{1}{2} \frac{r'^2 - 2rr' \cos \theta}{r^2} + \frac{1}{2} \left(\frac{1}{2} - 1 \right) \frac{(r'^4 - 4rr'^3 \cos \theta + 4r^2 r'^2 \cos^2 \theta)}{r^4} + \dots \right]$$

$$R = r + \frac{1}{2} \frac{r'^2 - 2rr' \cos \theta}{r} - \frac{1}{8} \frac{(r'^4 - 4rr'^3 \cos \theta + 4r^2 r'^2 \cos^2 \theta)}{r^3} + \dots$$

$$= r + \frac{r'^2}{2r} - r' \cos \theta - \frac{(r'^4 - 4rr'^3 \cos \theta + 4r^2 r'^2 \cos^2 \theta)}{8r^3} + \dots$$

$$= r - r' \cos \theta + \frac{r'^2}{2r} - \frac{(r'^4 - 4rr'^3 \cos \theta + 4r^2 r'^2 \cos^2 \theta)}{8r^3} + \dots$$

$$R = r - \hat{r} \cdot \vec{r}' + \frac{r'^2}{2r} - \frac{r'^4}{8r^3} + \frac{r'^3 \cos \theta}{2r^2} - \frac{r'^2 \cos^2 \theta}{2r} \dots$$

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So, then it takes a little while to work it out especially because it is always easy to make a careless mistake somewhere and get a wrong power somewhere. And then, you mess it up and spend another five minutes figuring out where it was, or two minutes trying to do it all over again. And we save all that time by skipping over this. So, all this is homework for you. You will work it out. It is already here but then these, follow these blue arrows, skip it. (Refer Slide Time: 35:31)

$$R = r - \hat{r} \cdot \vec{r}' + \frac{r'^2}{2r} - \frac{r'^4}{8r^3} + \frac{r'^3 \cos \theta}{2r^2} - \frac{r'^2 \cos^2 \theta}{2r} \dots$$

$$R = r - \hat{r} \cdot \vec{r}' + \frac{r'^2}{2r} (1 - \cos^2 \theta) - \frac{r'^4}{8r^3} + \frac{r'^3 \cos \theta}{2r^2} \dots$$

$$= r - \hat{r} \cdot \vec{r}' + \frac{r'^2 \sin^2 \theta}{2r} - \frac{r'^4}{8r^3} + \frac{r'^3 \cos \theta}{2r^2} \dots$$

$$= r - \hat{r} \cdot \vec{r}' + \frac{(\hat{r} \times \vec{r}')^2}{2r} + \dots$$

$$\frac{e^{ikR}}{R} \simeq \frac{e^{ik \left(r - \hat{r} \cdot \vec{r}' + \frac{r'^2 \sin^2 \theta}{2r} \right)}}{r - \hat{r} \cdot \vec{r}' + \frac{r'^2 \sin^2 \theta}{2r}}$$

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And here again, right because there are all these unless you combine the terms and take factor out the common terms and so on. Basically, that is high school mathematics. So, I do not want to spend any time working it out. But I am sure that, all of you can see at a glance what the logic is. And during the class, I want you to focus on the logic, okay.

And work out these intermediate steps on your own instead of watching a movie, for example, okay. (Refer Slide Time: 36:06)

$$\frac{e^{ikR}}{R} \approx \frac{e^{ik\left(r - \hat{r} \cdot \vec{r}' + \frac{r'^2 \sin^2 \theta}{2r}\right)}}{r - \hat{r} \cdot \vec{r}' + \frac{r'^2 \sin^2 \theta}{2r}}$$

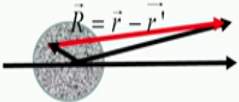
$$\frac{e^{ikR}}{R} \approx \frac{e^{ikr} e^{-ik(\hat{r} \cdot \vec{r}')} e^{ik\left(\frac{r'^2 \sin^2 \theta}{2r}\right)}}{r \left(1 - \frac{\hat{r} \cdot \vec{r}'}{r} + \frac{r'^2 \sin^2 \theta}{2r^2}\right)}$$

$$\frac{e^{ikR}}{R} \approx \frac{e^{ikr}}{r} e^{-ikr' \cos \theta} e^{\frac{ikr'^2 \sin^2 \theta}{2r}} \left(1 - \frac{\hat{r} \cdot \vec{r}'}{r} + \frac{r'^2 \sin^2 \theta}{2r^2}\right)^{-1}$$

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So, here, we now have an expansion. And then look at how these terms pop up. So, you have got terms and 1 over r and then one over r cube and then one over r square and so on right. So, now you can see how an approximation can be developed and you have much to do to rearrange these terms.

I mean 3 or 3 or 4 or 5 slides which I am skipping as you can see, okay. But it is very straightforward rearrangement of terms. So, I will leave it for you to work it out. (Refer Slide Time: 36:45)

$$\frac{e^{ikR}}{R} \approx \frac{e^{ikr}}{r} e^{-ikr' \cos \theta} e^{\frac{ikr'^2 \sin^2 \theta}{2r}} \left(1 - \frac{\hat{r} \cdot \vec{r}'}{r} + \frac{r'^2 \sin^2 \theta}{2r^2}\right)^{-1}$$


$$\frac{e^{ikR}}{R} \approx \frac{e^{ikr}}{r} e^{-ikr' \cos \theta} e^{\frac{ikr'^2 \sin^2 \theta}{2r}} \left(1 - \frac{r' \cos \theta}{r} + \frac{r'^2 \sin^2 \theta}{2r^2}\right)^{-1}$$

$$\frac{e^{ikR}}{R} \approx \frac{e^{ikr}}{r} e^{-ikr' \cos \theta} \left\{ 1 + \frac{ikr'^2 \sin^2 \theta}{2r} + \frac{1}{2} \left(\frac{ikr'^2 \sin^2 \theta}{2r} \right)^2 + \dots \right\} \left\{ 1 + \frac{r' \cos \theta}{r} - \frac{r'^2 \sin^2 \theta}{2r^2} + \dots \right\}$$

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I think it is more than three or four. But that is all right. I can always say it was only two slides. Are you all comfortable? Good. (Refer Slide Time: 36:58)

$$\frac{e^{ikR}}{R} = \frac{e^{ikr}}{r} e^{-ikr' \cos \theta} \left\{ 1 + \frac{ikr'^2 \sin^2 \theta}{2r} + \frac{1}{2} \left(\frac{ikr'^2 \sin^2 \theta}{2r} \right)^2 + \dots \right\} \left(1 + \frac{r' \cos \theta}{r} - \frac{r'^2 \sin^2 \theta}{2r^2} + \dots \right)$$

$$\frac{e^{ikR}}{R} \underset{r \rightarrow \infty}{\approx} \frac{e^{ikr}}{r} e^{-ik_f \cdot \vec{r}'}$$

Eq. 5.36 page 118
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Source point \vec{r}' Field point \vec{r}
 $\vec{R} = \vec{r} - \vec{r}'$ $\hat{k}_f = \hat{r}$
 $k\hat{r} = k\hat{k}_f = \vec{k}_f$

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So, here we are. So, we have the end result. What is the end result? That you have terms in 1 over $r + 1$ over r square and so on. And if you now retain only the leading term, okay only the leading term; because as r tends to infinity, you can always ignore 1 over r cube compared to 1 over r squared.

And you can always ignore one over r square with compared to 1 over r , okay. So, keep the leading terms; that is what the asymptotic region is about. And this is where the field point is, where the detector is. That is where you are carrying out the measurements. That is the place where you want to know what the solutions will turn out to be like. And in this limit as r tends to infinity, you have an ie to the ikR by R .

And yes we have met this term in our first course in quantum mechanics and in our early discussions in scattering theory. So, we are beginning to see a form that we know how to exploit and then we have some remaining terms.
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$$\psi_{\vec{k}_i}^+(\vec{r}) = \phi_{\vec{k}_i}(\vec{r}) + \iiint d^3\vec{r}' G_0^+(k, \vec{r}, \vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^+(\vec{r}')$$

$$\frac{e^{ikR}}{R} \underset{r \rightarrow \infty}{\approx} \frac{e^{ikr}}{r} e^{-i\vec{k}_f \cdot \vec{r}'} \quad \left[G_0^+(R) = \frac{-e^{ikR}}{4\pi R} \right]$$

$$\psi_{\vec{k}_i}^+(\vec{r}) = (2\pi)^{-3/2} e^{i\vec{k}_i \cdot \vec{r}} - \frac{1}{4\pi} \iiint d^3\vec{r}' \frac{e^{ikr}}{r} e^{-i\vec{k}_f \cdot \vec{r}'} U(\vec{r}') \psi_{\vec{k}_i}^+(\vec{r}')$$

Source point \vec{r}' Field point \vec{r}
 $\vec{R} = \vec{r} - \vec{r}'$ $\hat{k}_f = \hat{r}$
 $k\hat{r} = k\hat{k}_f = \vec{k}_f$

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So, you have got this e to the ik r by r and e to the -ikf dot r prime. So, this will go where e to the ikr by r goes. So, this is the e to the ikR by R. So, the minus sign is here. So, that comes here okay. The one over 4 pi is there, that comes over here. 1 over 4 pi then you have this e to the ik r by r which is good.

And this e to the ik r by r we know we can factor it outside the integration, because the integration is over the variable r prime which is changing for different source points in the scattering region. But they are all causing an effect at only one field point which is r. And that does not change as you integrate over r prime, okay.

The integration is over the source points for a given field point. So, e to the ik r by r can also be factored out. So, we will do that very quickly, now.
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$$\psi_{\vec{k}_i}^+(\vec{r}) = (2\pi)^{-3/2} e^{i\vec{k}_i \cdot \vec{r}} - \frac{1}{4\pi} \iiint d^3\vec{r}' \frac{e^{ikr}}{r} e^{-i\vec{k}_f \cdot \vec{r}'} U(\vec{r}') \psi_{\vec{k}_i}^+(\vec{r}')$$

$$\psi_{\vec{k}_i}^+(\vec{r}) = (2\pi)^{-3/2} \left[e^{i\vec{k}_i \cdot \vec{r}} + \frac{e^{ikr}}{r} \left(-2\pi^2 \right) \iiint d^3\vec{r}' \frac{1}{(2\pi)^{-3/2}} e^{-i\vec{k}_f \cdot \vec{r}'} U(\vec{r}') \psi_{\vec{k}_i}^+(\vec{r}') \right]$$

$$\psi_{\vec{k}_i}^+(\vec{r}) = (2\pi)^{-3/2} \left[e^{i\vec{k}_i \cdot \vec{r}} + \frac{e^{ikr}}{r} f(\hat{k}_i, \hat{k}_f) \right]$$

Scattering amplitude

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So, now we have got this e to the ik r by r outside. And then, we have this 4 pi to be properly accommodated. So, that has been done rather significantly, so that, you can get a plane wave

over here with a useful normalization, because but it does not matter what the normalization is, in the end, the normalization can be factored out.

So, now you have this $e^{i\mathbf{k}\cdot\mathbf{r}}$. This is the incident plane wave. And we know that a scattering solution we are in our very first what I call is a phenomenological solution, okay. The phenomenological solution of the scattering problem is what would you expect? That you it will be a superposition of the incident plane wave plus a scattered wave which is a spherically outgoing wave, right.

And the conservation of flux tells us that since the area of the sphere increases as r^2 as $4\pi r^2$ the amplitude will diminish as $1/r$. So, you factor out this $1/r$. So, that is over here. Then, you have got a spherical wave which is outgoing. Why is it out going? Because there is an $e^{-i\omega t}$ time dependence so you have factored that out.

And what is the rest of it? That is an angle dependent scattering amplitude, right. So, that is the scattering amplitude f that we have used in the phenomenological solution of the scattering problem. So, now we have got the solution to the scattering problem in a form that we have been using all along, okay.

And we have obtained it using the Lippman Schwinger equation. We know that the form is correct. We know that it gives us what we want. Except that we do not really know how to evaluate this integral, because the integral has got this $i\epsilon$ which is there on the left-hand side. So, we are going to have to worry about that.

But at least we have addressed one of the two issues which I mentioned. That we have to seek the asymptotic form because that is where the detector is and the other factor is. How to address this issue? So, we will do that so this is the scattering amplitude.
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f : Scattering amplitude


$$f(\hat{k}_i, \hat{k}_f) = -2\pi^2 \iiint d^3\vec{r}' \frac{1}{(2\pi)^3} e^{-i\vec{k}_f \cdot \vec{r}'} U(\vec{r}') \psi_{\vec{k}_i}^+(\vec{r}')$$

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$$f(\hat{k}_i, \hat{k}_f) = -2\pi^2 \iiint d^3\vec{r}' \phi_{\vec{k}_f}^-(\vec{r}') U(\vec{r}') \psi_{\vec{k}_i}^+(\vec{r}')$$

? ↓

$$= -2\pi^2 \langle \phi_{\vec{k}_f}^- | U | \psi_{\vec{k}_i}^+ \rangle = -\left(\frac{2\pi}{\hbar}\right)^2 m \langle \phi_{\vec{k}_f}^- | V | \psi_{\vec{k}_i}^+ \rangle$$



$$f(\hat{k}_i, \hat{k}_f) = -m \left(\frac{2\pi}{\hbar}\right)^2 T_{fi} \text{ Transition matrix element } \frac{d\sigma}{d\Omega} = m^2 \left(\frac{2\pi}{\hbar}\right)^4 |T_{fi}|^2$$

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

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And this is the solution I have used Joachain's Quantum theory of Collisions for this discussion. So, it is a very nice book that you will find very useful. And this term is nothing but the plane wave. So, this scattering amplitude I write as an integral of which the first factor is the plane wave corresponding to the wave vector k_f , because the wave vector here is k_f , mind you.

Over here, it is k_i that is the incident direction. The k_f exit direction is different. So, you must remember that. So, this is the k_f here, this is the k_i , with the incident wave vector. But this is the complete solution to the target scattering with the superscript pass which we do not know as yet. But we know that formally it is correct; it is acceptable, right.

So, this I have written in the Dirac notation. And this is in terms of the reduced potential. We can write it in terms of the physical potential V , which is why, the 2π in the \hbar cross and the m pop up one more time which we had eliminated. So, now in terms of the real physical potential, it is this.

And this is where I will conclude today's class. And we will take it from here tomorrow to determine, how we are going to deal with this problem, okay; because we have got a solution, all right. But it only gives us the solution in terms of the problem. Now, that is not very good, okay, so that we will discuss tomorrow or in the next class.

And this matrix element is often referred to as the transition matrix element. So, the scattering amplitude is proportional to the transition matrix element which is T and the differential cross section is just the modular square of the scattering amplitude as we have discussed earlier.

So, you get the model square of this. So, I will be happy to take a few questions. Otherwise, we will discuss what to do about this cheating, if you might want to call it, which is to give a solution in terms of the problem. But then, there are ways of handling it which is what we will discuss in the next class.