

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

Lecture 35
Coulomb scattering

Greetings, so today is the third lesson of this unit 5 and with this we will be concluding unit 5 and we will discuss Coulomb scattering. So, let me first of all tell you what the main references for this portion are. I will be using Sakurai's modern quantum mechanics mostly and you will find a very strong overlap also with the discussion in Landau Lifshitz book non relativistic quantum mechanics.


And before I begin, I think the today's class will be some sort of a tribute to Galileo who had nothing to do with the Coulomb interaction nor did he have anything to do with quantum scattering. But he did say one thing which is very remarkable that mathematics is the language of physics and you will see it in action in this class.

So, what will happen is that you know a lot of times one can when uses the language of mathematics to solve problems in physics. And it is important to be governed by the rigor in mathematics and continue to enjoy the charm and beauty in physics. So, one can very easily get lost in mathematics but one cannot ever compromise the rigor in mathematics. So, it is important to maintain the rigor but keep the focus on the physics of the problem.

So, this topic will require a little bit of mathematical analysis nothing very difficult or anything it is within the realm of you know B.Sc mathematics or what you do in mathematical methods and physics in your M.Sc courses. But the manipulation sometimes can take time. And I do not intend to spend all that time because this whole discussion is something that we will be concluding in just one class.

So, I have worked out all the major mathematical steps which are involved in the manipulation of the methodology. But I will not be discussing all of it in details in the class it will be there in the PDF which will be uploaded at the course webpage. So, you can always refer to that. But other than that I will probably skip some of the discussion on showing on demonstrating how those mathematical manipulations are done.

(Refer Slide Time: 03:16)



$$\left[\frac{(-i\hbar\nabla)^2}{2m} - \frac{(Z_1e)(Z_2e)}{r} \right] \psi(\vec{r}) = E\psi(\vec{r}) \quad \left| E = \frac{\hbar^2 k^2}{2m} > 0 \right.$$

$$\left[\nabla^2 + k^2 + \frac{2\gamma k}{r} \right] \psi(\vec{r}) = 0 \quad \left| m = \frac{m_1 m_2}{m_1 + m_2} \right.$$

$$\gamma = \frac{Z_1 Z_2 e^2 m}{\hbar^2 k} = \frac{Z_1 Z_2 e^2 m}{\hbar p} = \frac{Z_1 Z_2 e^2}{\hbar v} = \frac{\alpha c Z_1 Z_2}{v} \quad \left| \alpha = \frac{e^2}{\hbar c} \right.$$

$\gamma > 0 \leftrightarrow$ attraction

$(x, y, z) \rightarrow (\rho, \phi, z) \rightarrow (r, \theta, \phi)$

Cartesian	Cylindrical Polar	Spherical Polar
	$\rho^2 + z^2 = r^2$	
	$\rho^2 = r^2 - z^2 = (r+z)(r-z)$	

$\rightarrow (z, w, \phi)$
 Parabolic coordinates
 $w = r - z$
 $= r(1 - \cos \theta)$

74

PCO STITACS Unit 5 Quantum Theory of Collisions - Part 2

So, let us discuss the Coulomb scattering and this is the Schrodinger equation that we have to solve. So where is the cursor here it is. So this is the Schrodinger equation and this is the Coulomb interaction between two charged particles $Z_1e + Z_2e$. And in the case of the hydrogen atom it is just an electron and a proton right. So, this is the Schrodinger equation that you want to solve for continuum states.

Bound states we have done in our previous course of the Coulomb problem right, so this time we will discuss the Coulomb problem for the continuum. So, the energy is positive and you can rewrite it you know get rid of this m and \hbar cross and so on and it simplifies to this. So, this is the 1 over r Coulomb interaction and γ takes care of all these other constants. So, this is what γ turns out to be okay.

So, this is the straight forward substitution and rewriting the Schrodinger equation in a convenient form. Now γ whenever it is positive you talk about an attractive interaction and in the electron photon system the hydrogen that is what it is. Now we could use any coordinate system one could use the Cartesian coordinates or cylindrical polar or spherical polar.

And you always choose a coordinate system which is well adapted to the symmetry of the Hamiltonian. And what we did in the previous course or in our first course in quantum mechanics or in atomic physics we solve the problem in spherical symmetry because obviously the Coulomb interaction is which goes as 1 over r has got a spherical symmetry. So, that is the appropriate coordinate system of choice.

The Coulomb interaction however has another symmetry that you have a to center interaction right. So, you have got to charge particles and there is an interaction between these two, so

there is as azimuthal symmetry about the line joining these two particles. So, there is an azimuthal symmetry and one could use a coordinate system in which one has as azimuthal symmetry.

And of course the spherical symmetry includes this, so the spherical polar coordinate system has got this r theta and Phi, Phi is the azimuthal angle, so that is fine enough. But not just a spherical polar, you also have the parabolic coordinates okay. Because the parabola also has got an axis of symmetry okay so one can use the parabolic coordinates as well for this problem.

And if you just look at these relations, so Rho is the distance in the cylindrical polar coordinates r is the distance in the spherical polar, so I am using the usual notation. And one can introduce the parabolic coordinates as z, w, Phi which are independent degrees of freedom in which w is defined as r - z.

So, this is the parabolic coordinate system and the Coulomb problem can be solved also in the parabolic coordinate system. So, that is what we are going to do. (Refer Slide Time: 06:32)

$(x, y, z) \rightarrow (\rho, \phi, z) \rightarrow (r, \theta, \phi) \rightarrow (z, w, \phi)$
 Cartesian Cylindrical Polar Spherical Polar Parabolic coordinates
 $\rho^2 + z^2 = r^2$
 $\rho^2 = r^2 - z^2 = (r+z)(r-z)$
 $W = r - z$
 Introduce u
 $w \leftrightarrow \frac{-iu}{k}$
 $(z, w, \phi) \leftrightarrow \left(z, \frac{-iu}{k}, \phi \right) \leftrightarrow (z, u, \phi)$
 $\psi(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} \chi(u) = e^{ikz} \chi(u)$

NPTEL
 PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2
 75

So, let me spend a few minutes on this coordinate system, so this is the parabolic coordinates w is r - z. Now notice that these are degrees of freedom x,y,z are all independent of each other Rho, Phi, z said are independent of each other r theta phi are also independent of each other. And likewise these will also be independent of each other. So, these are the independent degrees of freedom.

One can also introduce a parameter u instead of w but u and w are just proportional to each other. And the information in w is the same as the information in u except that it is scaled by

a factor minus i over kh cross square k square. Yes (Question time: 07:12- not audible) yeah I am going to explain that I am going to come on that. It is independent yes it is absolutely independent.

So, w is -iu over k, so the information in w and u is essentially the same. And -i and k is just what is scaling it. So, you have a coordinate system in z, w, Phi or z, u, Phi and you know you can express your parabola coordinates either is z, w, Phi or z, u, Phi. So, they are completely equivalent to each other.

And then you can write the wave function as e to the ikz and a function of the variable u which is this you which is coming from w under Schrodinger equation the differential equation it will turn out is separable in the z and u coordinates. (Refer Slide Time: 08:14)

$(x, y, z) \rightarrow (\rho, \phi, z) \rightarrow (r, \theta, \phi)$
 ↑ ↑ Cartesian Cylindrical Polar Spherical Polar
 $x = r \sin \theta \cos \phi$ $x = (r \sin \theta) \cos \phi$
 $y = r \sin \theta \sin \phi$ $y = \frac{x}{\cos \phi} \sin \phi = x \tan \phi$
 $z = r \cos \theta$
 $(x, y, z) \rightarrow$ independent degrees of freedom
 $w = r - z = r(1 - \cos \theta)$ ↑ (z, w, ϕ) ↑ (z, u, ϕ)
 Parabolic coordinates
 $w \leftrightarrow -iu/k$
 NPTEL PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 76

Because that is the whole idea of simplifying your geometry, so yes about the independence of the coordinate system, so here you have got an example that x, y, z and Rho, Phi, z. So, you always have relations which give you the transformations from one coordinate system to another. You can always; basically a point in the 3 dimensional space is specified by three independent degrees of freedom.

And you can specify these three independent degrees of freedom but there is nothing sacred about one coordinate system or another and you can always carry out transformations from one to the other. So, let us take a typical example from the Cartesian coordinate system to the spherical polar coordinate system.

And these are the usual coordinate transformations and you can express the same point in space either as x, y, z or as r theta Phi and you have exactly the same information. Now

nobody disputes the fact that x , y , z are independent degrees of freedom okay. So, one does not vary with respect to the other and you need to specify the information about each of these three degrees of freedom to pin down where a point in the spaces right.

Now likewise these three z , w and Φ will also have to be specified or z equivalently z , u and Φ , now that does not stop you to have relationships between one coordinate system and another okay. So, let us take another example over here, so this is the relationship over here and here w is expressed in terms of z and which is what you observed okay. But said itself is just $r \cos \theta$ okay.

And you have is effectively what you have done is expressed w in terms of r and θ . So, there is nothing you know absurd or nothing mysterious about it because you always express like in this box you have already expressed x in terms of our θ Φ you can also observe now it what applies to w also applies to u because they are simply scaled with respect to each other but then essentially these are independent degrees of freedom.

And you can always write x as $r \sin \theta \cos \Phi$ but then you can do a little bit of algebraic manipulation and write $r \sin \theta$ is x over $\cos \Phi$. And then write y as $x \tan \Phi$. Now that does not; so you have written y in terms of x as such it does not make y dependent on x okay. These are independent degrees of freedom and they continue to be so.

So, that is precisely what is happening over here that z , u and Φ and z , w and Φ , the either the first set of the second set the 2 being completely equivalent. They are completely independent degrees of freedom that you happened to express one in terms of r - z does not make w dependent on z . And whenever you are taking the gradient or the laplacian or whenever you are taking the derivatives of any operator.

When you take the derivative with respect to w then you have to take a partial derivative with respect to w with nothing else happening to the other two coordinates okay. So, that is important to keep track of this so that you construct the correct gradient operator. And then of course it is a straightforward extension to get the Laplacian which is what you will have to do to write the Schrodinger equation.

Because in the Schrodinger equation you have got the ∇^2 operator. So, all you are going to do is to write the Schrodinger equation in the parabolic coordinates and now we know how to do that okay.

(Refer Slide Time: 11:59)

$W = r - z \quad (x, y, z) \leftrightarrow (z, u, \phi)$
 $(z, w, \phi) \leftrightarrow \text{Parabolic coordinates} \leftrightarrow (z, u, \phi)$

$$\frac{\partial}{\partial x} = \cancel{\frac{\partial z}{\partial x}} \frac{\partial}{\partial z} + \frac{\partial w}{\partial x} \frac{\partial}{\partial w} + \frac{\partial \phi}{\partial x} \frac{\partial}{\partial \phi}$$

$\tan^{-1}\left(\frac{y}{x}\right) = \phi \quad \frac{\partial \phi}{\partial x} ? \quad \psi(\vec{r}) = e^{ik \cdot \vec{r}} \chi(u) \quad \frac{\partial \psi}{\partial \phi} = 0$
 $= e^{ikz} \chi(u)$

Our interest: functions which are azimuthally symmetric (cylindrical / parabolic)

$$\frac{\partial}{\partial x} \equiv \frac{\partial w}{\partial x} \frac{\partial}{\partial w}$$

PCD SITACS Unit 5 Quantum Theory of Collisions - Part 2 77

So, let us find what the partial derivative operators are so that we can write the Schrodinger equation and the del square operator. So, here these are independent degrees of freedom and you can write the partial derivative because you can certainly go from the spherical polar to the parabolic coordinates or if you like further from the Cartesian to the parabolic it does not matter.

And here you can; here you see how you go from the Cartesian coordinate system to the parabolic coordinate system. So, you can write the partial derivative operator del by del x and then you will need in the laplacian the del2 by del x2 and so on right. So, those are the operators you will have to construct, so you can use the chain rule because there are three degrees of freedom.

So, there will be these three terms it does not mean that all of them are going to contribute because z we already know is independent of x right. So, the first term will certainly not contribute. And then you may have the possibility of getting find you know find out how Phi varies with respect to x and get that partial derivative. And you have the relation already between Phi and as tan inverse of y over x.

So, you can go ahead and determine del Phi by del x but you do not even have to do that why should you because the coordinate system that you are using is our interest in doing this problem is to apply to a specific two body problem. The two body problem which increases is the Coulomb interaction.

You have got to charge particles and they are interacting along the line joining them. So, there is as a little symmetry about it right. So, because of this symmetry you will not find any dependence of the solutions on the azimuthal angle Phi in the parabolic coordinate system.

So, this ϕ is the same as the Φ of the spherical polar coordinate system or the cylindrical polar coordinate system it is the same as azimuthal angle.

And there will be no dependence on that. So, the wave function will be independent of Φ because of this as azimuthal symmetry. And this term because this is in any case an operator but it is not going to operate on an arbitrary function of space. It is intended eventually to operate on the wave function for a system which has got an inbuilt symmetry. And this in built symmetry of the Coulomb interaction is of central interest to us okay.

Given that the third term also does not have to be taken into account because any derivative with respect to Φ is of no interest for the Coulomb problem which is the two-body problem which has got an as azimuthal symmetry. What does it give us for the partial derivative operator ∇ over ∇x , it gives us only the middle term which is ∇w by ∇x and then ∇ over ∇w right.

So, this is the only term that we really need to worry about even when you take the first order partial derivatives okay. And it will be the same when you take the second order partial derivatives when you construct the laplacian.
(Refer Slide Time: 15:19)

$W = r - z \quad (z, w, \phi) \leftrightarrow \text{Parabolic coordinates}$

$\frac{\partial}{\partial x} \equiv \frac{\partial w}{\partial x} \frac{\partial}{\partial w}$ since $\frac{\partial \psi}{\partial \phi} = 0$ & $(x, y, z) : \text{independent}$

$w = (x^2 + y^2 + z^2)^{\frac{1}{2}} - z$

$\Rightarrow \frac{\partial w}{\partial x} = \frac{1}{2}(r^2)^{-\frac{1}{2}}(2x) = \frac{x}{r}$

$\frac{\partial}{\partial x} \equiv \frac{x}{r} \frac{\partial}{\partial w}$

PCO STITACS Unit 5 Quantum Theory of Collisions - Part 2

So, now you have got the operator ∇ over ∇x , x , y and z are independent and likewise z , w and Φ are also independent of each other. Yes there is a relationship between w and z which is basically a relationship which describes w in terms of the spherical polar coordinates r and θ okay, so that is that is the basic relationship. So, that there is nothing very mysterious about it.

So, now let us get this del w by del x which you can get very easily from here. And that gives del w by del x to be x over r. And this is what I mentioned that all these intermediate steps I will not comment on in the class because they are straight forward you know very simple mathematical manipulations they are important. And it is important to do it rigorously but I will not be spending time commenting on those.

But they will all be there in the slides and you can refer to those intermediate steps in the PDF when it is uploaded at the course webpage. So, this partial derivative del w by del x is x over r and that gives us the operator del over del x in terms of del over del w it has to be scaled by x over r. So, this is your partial derivative operator for del over del x. (Refer Slide Time: 16:44)

$$\frac{\partial^2}{\partial x^2} = \left(\frac{x^2}{r^2} \frac{\partial^2}{\partial w^2} \right) + \left(\frac{1}{r} - \frac{x^2}{r^3} \right) \frac{\partial}{\partial w} \quad \boxed{\frac{\partial}{\partial x} = \frac{x}{r} \frac{\partial}{\partial w}}$$

$$\frac{\partial^2}{\partial y^2} = \left(\frac{y^2}{r^2} \frac{\partial^2}{\partial w^2} \right) + \left(\frac{1}{r} - \frac{y^2}{r^3} \right) \frac{\partial}{\partial w} \quad \boxed{\psi(\vec{r}) = e^{ikz} \chi(u)}$$

$$\frac{\partial^2}{\partial z^2} = \left(\frac{w^2}{r^2} \frac{\partial^2}{\partial w^2} \right) + \left(\frac{w}{r^2} - \frac{w^2}{r^3} \right) \frac{\partial}{\partial w} - \frac{2w}{r} \frac{\partial^2}{\partial z \partial w} + \frac{w}{r^2} \frac{\partial}{\partial w} + \frac{\partial^2}{\partial z^2}$$

$$w \leftrightarrow \frac{-iu}{k} \quad \frac{\partial}{\partial w} \equiv \frac{\partial}{\partial \left(\frac{-iu}{k} \right)} \equiv ik \frac{\partial}{\partial u}$$

NPTEL
PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2
79

And now you can get the second derivative and you can carry on the same extension, so you know how to do that okay. So, this will give you the second derivative you can likewise get the derivative with respect to y and also with respect to z. So, all the derivatives with respect to x, y and z are now expressed in terms of derivatives with respect to z and w. So, z w Phi these are the three independent degrees of freedom.

And your partial derivatives with respect to x, y, z are written in terms of partial derivatives with respect to w or z okay. The dependence on Phi has already been taken care of by the symmetry of the interaction itself. So, the hydrogen atom the Coulomb problem has got a very peculiar symmetry and we know that it has this s or 4, symmetry which we have discussed in our previous course.

And as a result of that it becomes possible to solve it not just in the spherical polar coordinate system but also in another coordinate system which is the parabolic quadrant system. So, that is the solution that we will discuss. So, these are your coordinates and now having

commented on the coordinate system you can write the derivative operator with respect to w in terms of derivative operator with respect to u .

Because u and w have got this scaling relationship okay. There is of course this k over here which is the velocity kind of term right but it is not a space dependent term. So, so far as variations with respect to spatial coordinates are concerned it is a constant. So, now in this coordinate system this Schrodinger wave function is separable in the z and u coordinates. So, this is a matter of detail which I will not comment on or work out in details in the class. (Refer Slide Time: 18:39)

$$(z, w, \phi) \leftrightarrow \left(z, \frac{-iu}{k}, \phi\right) \leftrightarrow (z, u, \phi)$$

$$\left[\nabla^2 + k^2 + \frac{2\gamma k}{r}\right] \psi(\vec{r}) = 0$$

Azimuthal symmetry about the 2-center coulomb interaction.

Schrodinger equation is separable in z and u coordinates

$$\psi(\vec{r}) = e^{ikz} \chi(u)$$

$$\left[u \frac{d^2}{du^2} + (1-u) \frac{d}{du} - i\gamma\right] \chi(u) = 0$$

NPTEL
 PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2
 80

But exploiting this as azimuthal symmetry this will not be possible for an arbitrary function of space because that the dependence on ϕ and x that term will have to be taken care of but you do not have to do that for this particular symmetry. So, here you separate out the Schrodinger equation in z and you and get all the dynamics in just one equation which is the differential equation in the coordinate u okay.

Now this the you have done this with so many three dimensional problems in which you wind up exploiting the symmetry and then reduce the Schrodinger equation to a one dimensional Schrodinger equation like the radial Schrodinger equation. All the dynamics is then there in the radial Schrodinger equation all the spherical symmetry is taken care of by the spherical harmonics and so on right.

So, that is what we did in a you know in our in introductory courses and quantum mechanics and atomic physics. So, here you have got the entire dynamics in this one dimensional equation this is not a radial equation because it is it does not have the radial symmetry anymore it does not have the spherical symmetry anymore. It has got the parabolic symmetry okay. So this is written in terms of the parabolic coordinates.

And not surprisingly you do not have anything that looks like the centrifugal term which is that $l(l+1)$ by r square which I am sure all of you remember in the radial equation because l is not a good quantum number angular momentum is not conserved. There is no spherical symmetry over here.

So, you do not have that term instead you have a differential equation in the variable u . And this is the differential equation which we must solve to get the solutions of the Coulomb problem okay.

(Refer Slide Time: 20:42)

$$\left[\nabla^2 + k^2 + \frac{2\gamma k}{r} \right] \psi(\vec{r}) = 0$$

Schrodinger equation for the coulomb problem

$$\left[u \frac{d^2}{du^2} + (1-u) \frac{d}{du} - i\gamma \right] \chi(u) = 0$$

$r \rightarrow \infty$ asymptotic solutions

Away from the forward ($\theta=0$) direction

$$u = ik(r-z) \rightarrow ikr ; u \rightarrow \infty$$

Explore the solution: $\chi(u) \simeq u^\beta$

NPTEL
PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 81

So, let us proceed to get this solution now. So this is the Schrodinger equation for the Coulomb problem and again we are not interested in very detailed solutions because our interest in collision physics is to seek solutions in the asymptotic region okay. You as r tend to infinity or in this case u will go to infinity right.

So, that is the asymptotic region because as r goes to infinity u will go to infinity. So, this is the region of interest and this will typically be away from the forward direction right theta because z is $r \cos \theta$. So, when theta is $\pi/2$, this term will go to 0 and then u becomes ikr and then you can get the asymptotic limit. So, now we have to find a solution, so what we will do is we will propose some solution and figure out if it is an acceptable solution okay.

So, we propose we explore the possibility of having a solution which goes as a u^β power of u , β is something that we will find out. And again we will make use of techniques in complex analysis which we used in our first class of this unit also for the Lippmann Schwinger equation. We do use contour integration and that is a very powerful technique which we will use in today's class as well.

(Refer Slide Time: 22:12)

$$\left[u \frac{d^2}{du^2} + (1-u) \frac{d}{du} - i\gamma \right] \chi(u) = 0 \quad \chi(u) \approx u^\beta$$

$$u = ikw = ik(r-z)$$

$$\frac{d}{du} \chi(u) \approx \beta u^{\beta-1} \quad ; \quad \frac{d^2}{du^2} \chi(u) \approx \beta(\beta-1)u^{\beta-2}$$

$$u \frac{d^2 \chi(u)}{du^2} - u \frac{d \chi(u)}{du} + \frac{d \chi(u)}{du} - i\gamma \chi(u) \approx 0$$

$$\left[u\beta(\beta-1)u^{\beta-2} + (1-u)\beta u^{\beta-1} - i\gamma u^\beta \right] \approx 0$$

$$\left[\beta(\beta-1)u^{\beta-1} + (\beta u^{\beta-1} - \beta u^\beta) - i\gamma u^\beta \right] \approx 0 \quad i\gamma + \beta = 0$$

$$\left[\beta^2 u^{\beta-1} - \beta u^{\beta-1} + \beta u^{\beta-1} - \beta u^\beta - i\gamma u^\beta \right] \approx 0$$

$$\left[\beta^2 u^{\beta-1} - (i\gamma + \beta) u^\beta \right] \approx 0 \quad \beta = -i\gamma$$

Solution for arbitrary u requires that

NPTEL PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 82

Now we have got the differential equation in the variable u and we have proposed the solution χ which goes as u to the power β . So, we can take the first derivative which will be βu to the power $\beta - 1$. Now we can take the second derivative right and put the corresponding terms from the right-hand side of these two equations in this differential equation and see what we get.

So, here we have done that and you can see that this term has come we will have to go here. In the second derivative of χ with respect to u , the first derivative will have to come here okay. So, put in all of these terms, so here you have our two terms one is d by du and the other is $-u$ times d by du , so $-u$ times d by du is here okay. And the other term with the coefficient 1 is here.

So, all you have done is to substitute a solution which is χu which goes as u to the power β okay. There may be some constants which multiply that but let them be because any solution multiplied constant is always an acceptable solution, so we can take care of it in normalization and so on. So, now you plug in these the right-hand sides in the first and the second derivatives.

And I will not comment on that I this is something for you to work out yourself but all of that is worked out over here and it will be there in the PDF file which will be uploaded at the course webpage. So, you substitute all of these combine the terms find out if there is anything which cancels with anything else right. Combine all the terms so that is a straightforward manipulation I will not spend any time commenting of that.

And bring you to the main result which is here so your relation boils down to two terms u to the power $\beta - 1$ and one goes as u to the power β of which in the asymptotic region this will be the leading term. And this being the leading term we need to find the condition under which the term will go to 0 okay. On the right hand side you have got a zero, so if we can ensure that the leading term goes to 0.

So, when will the leading the equation with the leading term go to 0 when $i\gamma + \beta$ is 0 right. So, $i\gamma + \beta$ must be 0 and this is this condition will make it possible there may be some additional conditions have to be satisfied and we are going to discuss those. So, this will be the situation under which we can accept a solution for χ which goes as u to the power β .

And the complete solution of course is e^{ikz} times χ which we have written in the previous slide right. So this is your solution now to the Schrodinger equation this is one solution we need one more right.

(Refer Slide Time: 25:25)

$$\left[u \frac{d^2}{du^2} + (1-u) \frac{d}{du} - i\gamma \right] \chi(u) = 0$$

$$\chi(u) \rightarrow u^{-i\gamma} \rightarrow \{k(r-z)\}^{-i\gamma}$$

$$\chi(u) \rightarrow [e^{\ln\{k(r-z)\}}]^{-i\gamma}$$

$$\chi(u) \rightarrow e^{-i\gamma \ln\{k(r-z)\}}$$

$$\psi(\vec{r}) = e^{ikr \cos \theta} \chi(u) = e^{i[kz - \gamma \ln\{k(r-z)\}]}$$

$$\psi_{\uparrow}(\vec{r}) \rightarrow e^{i[kz - \gamma \ln\{k(r-z)\}]}$$

$$\left. \begin{array}{l} \psi(\vec{r}) = e^{ik \cdot \vec{r}} \chi(u) \\ \chi(u) \simeq u^{\beta} \\ \beta = -i\gamma \end{array} \right\}$$

NPTEL
 PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2
 83

So, we need one more so let us have a look at this solution this is the first solution your solution is a product of χ and this function of z which is e^{ikz} right $r \cos \theta$ is that is kz . So, this is one solution and in this solution now χ goes as u to the power β . We have agreed that β will have to be $-i\gamma$, so you put $-u$ to the power $-i\gamma$ over here and χ goes as $kr - z$ to the power $-i\gamma$.

Now again a little bit of manipulation is called for. And again I have followed like I pointed out the treatment in the book by Sakurai in fact this topic was not originally included in Sakurai's book. And it is often left out in many M.Sc courses in on quantum mechanics or

atomic physics but I think it is a nice thing to be done. So, this is you have u to the power $-i\gamma$, so you have got u is this.

So, let us write this $kr - z$ as e to the power logarithm which is the same thing right. So, this is a convenient manipulation and you will see how this manipulation makes it possible to exploit methods and complex analysis to get the solution for the Coulomb problem. So, the end result will turn out to be a very beautiful one and I want to get there without getting lost in mathematical manipulations.

But not avoiding the rigor in mathematics, so I would like to tell you what the major mathematical considerations are like I commented on the parabolic coordinates. I will do so for the rest of the class as well. But I will not work out every single transformation which will be there in the PDF.

So, this is what we get for χ and once you have it. You can write the solution as a product of e to the ikz times χ of u , so it goes as e to the ikz is here and then you have got the second term coming over here. So, this is one solution that you get and this being the first solution if have now put a subscript 1 over here.

To remind us that this is one of the solutions that we will use then we are going to look for one more okay. So, this is one solution that we have.
(Refer Slide Time: 28:18)

The slide contains the following mathematical content:

- Equation: $\left[u \frac{d^2}{du^2} + (1-u) \frac{d}{du} - i\gamma \right] \chi(u) = 0$ with a circled expression $u = ikw = ik(r - z)$.
- Text: "Explore another solution: $\chi(u) \approx u^\beta e^u$ "
- Equation in a box: $\left[\nabla^2 + k^2 + \frac{2\gamma k}{r} \right] \psi(\vec{r}) = 0$
- Derivation: $\frac{d}{du} \chi(u) = \beta u^{\beta-1} e^u + u^\beta e^u$
- Derivation: $\frac{d}{du} \frac{d}{du} \chi(u) = \frac{d}{du} (\beta u^{\beta-1} e^u) + \frac{d}{du} \chi(u)$
- Equation: $\frac{d^2}{du^2} \chi(u) = \{ \beta(\beta-1) u^{\beta-2} e^u + \beta u^{\beta-1} e^u \} + \{ \beta u^{\beta-1} e^u + u^\beta e^u \}$
- Equation: $\frac{d^2}{du^2} \chi(u) = \beta(\beta-1) u^{\beta-2} e^u + 2\beta u^{\beta-1} e^u + u^\beta e^u$

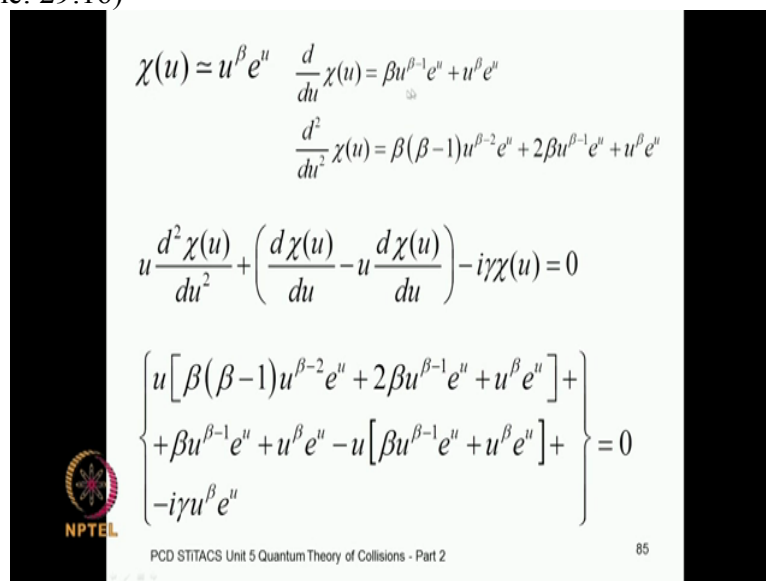
NPTEL logo is visible in the bottom left corner. Page number 84 is in the bottom right corner. Footer text: PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2

All right now let us look for another solution now this time we will look for a solution of this kind u to the power β multiplied by e to the power u . And let us see under what conditions this will be an acceptable solution will it be as an acceptable solution at all. Are there some conditions which will make this an acceptable solution.

And if it turns out that those conditions are met then what would the solution give us so far. As the solution of the collision problem is concerned because at the end of the day you want to get the scattering cross section okay scattering amplitude and things like that. So, those are the fundamental quantities of interest.

So, now again I will not spend any time commenting on this all I have done is to take this function of Chi taken the first derivative and the second derivative combined common terms adjusted the coefficients right.

(Refer Slide Time: 29:16)



$$\chi(u) \simeq u^\beta e^u \quad \frac{d}{du} \chi(u) = \beta u^{\beta-1} e^u + u^\beta e^u$$

$$\frac{d^2}{du^2} \chi(u) = \beta(\beta-1)u^{\beta-2} e^u + 2\beta u^{\beta-1} e^u + u^\beta e^u$$

$$u \frac{d^2 \chi(u)}{du^2} + \left(\frac{d\chi(u)}{du} - u \frac{d\chi(u)}{du} \right) - i\gamma \chi(u) = 0$$

$$\left\{ \begin{array}{l} u \left[\beta(\beta-1)u^{\beta-2} e^u + 2\beta u^{\beta-1} e^u + u^\beta e^u \right] + \\ + \beta u^{\beta-1} e^u + u^\beta e^u - u \left[\beta u^{\beta-1} e^u + u^\beta e^u \right] + \\ - i\gamma u^\beta e^u \end{array} \right\} = 0$$

PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 85

And I get a certain result which I am about to show you. So, this is what I get for the first derivative this is what I get for the second derivative I will not comment on how you go through this step-by-step. So, you have both the first and the second derivative which will now go into the Schrodinger equation or what is coming out of the Schrodinger equation which is the differential equation for Chi.

Which is a, which has got exactly the same information as that was there in the Schrodinger equation itself. And you put all of these terms for the first derivative for the second derivative you have got these three terms for here you have got these two terms.

(Refer slide Time: 30:03)

$$\begin{cases}
 u[\beta(\beta-1)u^{\beta-2}e^u + 2\beta u^{\beta-1}e^u + u^\beta e^u] + \\
 + \beta u^{\beta-1}e^u + u^\beta e^u - u[\beta u^{\beta-1}e^u + u^\beta e^u] + \\
 -i\gamma u^\beta e^u
 \end{cases} = 0$$

$$\begin{cases}
 \beta(\beta-1)u^{\beta-1}e^u + 2\beta u^\beta e^u + u^{\beta+1}e^u + \\
 + \beta u^{\beta-1}e^u + u^\beta e^u - \beta u^\beta e^u - u^{\beta+1}e^u + \\
 -i\gamma u^\beta e^u
 \end{cases} = 0$$

$u = ikr(1 - \cos\theta)$

$u = ikw = ik(r-z)$

$$\beta^2 u^{\beta-1} e^u + (\beta + 1 - i\gamma) u^\beta e^u = 0$$

$$\beta + 1 - i\gamma = 0$$

↑ Leading term in the asymptotic region

$$\beta = -1 + i\gamma \quad \chi(u) \approx u^\beta e^u$$

$$\chi(u) \approx u^{-1+i\gamma} e^u = \frac{1}{u} u^{i\gamma} e^u = \frac{1}{ik(r-z)} \{ik(r-z)\}^{i\gamma} e^{\{ik(r-z)\}}$$

86


PCD STIACS Unit 5 Quantum Theory of Collisions - Part 2

Put them all together find out if there is anything common what combines with what. Manipulate the common terms right that is very straightforward mathematical manipulation I will spend no time on that and this thing is struck okay here it is. So, now you see that okay some of these terms cancel each other right.

So, that is the kind of simple manipulation that is attempted over here. So, now what does it give us you get when you combine all the terms you find that the leading term in this case goes as u to the β in this. The other term is due to the $\beta - 1$, so this time you find that the proposed solution would be acceptable if this coefficient $\beta + 1 - i\gamma$ goes to 0 because that will make the that will set balance the equation the right hand side is 0.

So, now you have another condition here that $\beta + 1 - i\gamma$ which is the coefficient of the leading term, so this would go to zero. So, β if you take these two terms on the other side is $-1 + i\gamma$. And this is what you get for the second solution. So, you can write this again in terms of $r - z$ because u is nothing but ik times $r - z$.

So, you can write this either in terms of u or you can write it in terms of $ikr - z$ then instead of this u you have got $ikr - z$ to the power $i\gamma$ which is here and then you have got e to the power u which is e to the power $ikr - z$ okay, so pretty straightforward as such all right okay. (Refer Slide Time: 31:57)



$$\chi(u) \simeq \frac{1}{ik(r-z)} \{ik(r-z)\}^{i\gamma} e^{ik(r-z)}$$

$$\{k(r-z)\}^{i\gamma} = [e^{\ln\{k(r-z)\}}]^{i\gamma} = e^{i\gamma \ln\{k(r-z)\}}$$

$$\Rightarrow \chi(u) \simeq \frac{1}{k(r-z)} e^{i\gamma \ln\{k(r-z)\}} e^{ik(r-z)}$$

$$\psi_2(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \chi(u) = e^{ikz} \frac{e^{i\gamma \ln\{k(r-z)\}}}{k(r-z)} e^{ik(r-z)} = \frac{e^{i\{kr+\gamma \ln\{k(r-z)\}\}}}{k(r-z)}$$

$$\psi_2(\vec{r}) = \frac{e^{ikr}}{k(r-z)} e^{i\gamma \ln\{k(r-z)\}} \quad \text{outgoing wave} \quad e^{-i\omega t}$$

PCD 5TITACS Unit 5 Quantum Theory of Collisions - Part 2 87

So this is your solution for Chi, let us manipulate this similar to how we had done earlier. So, this $kr - z$, I write as e to the power logarithm of this term and this whole thing to the power i gamma. So, now it becomes e to the power i gamma log of $kr - z$ okay. What does it give us for Chi so you have this e to the power $ikr - z$ coming from here, so that is over here and the rest of the term are here.

So, this is our second solution which is e to the ikz times Chi of u . So, this is the second solution and you have to multiply this Chi of u with this e to the ikz and then you can again combine the terms in some fashion. Notice that you have got e to the $-ikz$ coming from here there is a $-z$ over here, so here there is an e to the $-ikz$ sitting that cancels this e to the ikz okay and the rest of the terms are here okay alright.

So, now we have got the second solution which is e to the ikr over $kr - z$ and this looks nice right because that is the kind of solution we are looking for okay. Absolutely that is exactly the kind of solution we are looking for because we know that there is a time dependence involved.

And the time dependence is included for stationary states by the term e to the $-i\omega t$ and when you put this e to the $-i\omega t$ together with this e to the ikr you have got outgoing waves and that is just the kind of solution you are looking for right in scattering in collision problems. So, however there are additional features like in the collision problems that we have discussed earlier.

And we discuss this in the very first unit of this course and we ruled out the application of those methods to the $1/r$ potential okay. I had mentioned that the Coulomb problem you cannot handle using those methods and the reason is because in the usual scattering solution

what multiplies the e to the ikr over r is the scattering amplitude and you do not have any our dependence there.

But here what is multiplying this blue box is there is a residual r dependence here okay. So, this is a peculiar feature of the Coulomb problem and it is because of the infinite tail that the Coulomb interaction has. The 1 over r goes all the way to infinity and no matter how far the two charges are okay. They will always interact with each other. It has got very fascinating implications like in collision physics.

You have got the scattering cross section which goes to 0 as k goes to 0 okay at the threshold. But the threshold photo ionization cross section as you know very well is always finite. It is because there is some interaction which is possible in fact even at infinite distance. So that is a very special feature of the Coulomb problem and we will have to figure out how to handle that. So, that is what the remaining discussion in this class will be.

(Refer Slide Time: 35:26)

$$\psi_1(\vec{r}) \rightarrow e^{i[kz - \gamma \ln\{k(r-z)\}]} \quad \psi_2(\vec{r}) = \frac{e^{i\{kr + \gamma \ln\{k(r-z)\}\}}}{k(r-z)}$$

$$\psi(\vec{r}) \rightarrow e^{i[kz - \gamma \ln\{k(r-z)\}]} + \tilde{f}_c(k, \theta) \frac{e^{i\{kr + \gamma \ln\{k(r-z)\}\}}}{k(r-z)}$$

$$r-z = r - r \cos \theta = r(1 - \cos \theta) = r \left(2 \sin^2 \frac{\theta}{2} \right)$$

$$\ln \{k(r-z)\} = \ln \left\{ kr \left(2 \sin^2 \frac{\theta}{2} \right) \right\} = \ln(2kr) + 2 \ln \sin \frac{\theta}{2}$$

$$\psi(\vec{r}) \rightarrow e^{i[\vec{k} \cdot \vec{r} - \gamma \ln\{kr - \vec{k} \cdot \vec{r}\}]} + \tilde{f}_c(k, \theta) \frac{e^{i\{kr + \gamma \ln(2kr) + 2\gamma \ln \sin \frac{\theta}{2}\}}}{k(r-z)}$$

NPTEL
PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2
68

So now these are the two solutions that we have okay. On the complete solution we can write as a superposition of these two scaled by some appropriate factor which will have the information of the scattering amplitude that we are looking for right. It will have energy dependence it will have theta dependence and I have written this factor which takes the role of the scattering amplitude.

But it is a matter of notation I am going to stay as close as possible to the notation which is used in the in Sakurai's book, Modern Quantum Mechanics in chapter 7. And he uses a scattering amplitude which is f_c whereas the f_c tilde which I have used is slightly different from that but I will tell you what the relationships are okay.

So, I have this term which is going to give us information about the scattering amplitude and the differential cross section. So, to get that first of all you recognize that $r - z$ is r times twice sine square half theta okay. So, again there are some simple trigonometric manipulations which will turn out to be very handy which I will again not spend too much time commenting on.

And instead of this $r - z$, I now have this twice sine square theta over 2 and now you can separate these two terms these are additive okay. You are taking the logarithm of this product so these two terms add up. And if you now see we will consider the solution which is a superposition of these two terms. And here instead of this $r - z$, I have exploited this twice sine square theta over 2.

And then this logarithm which is written as a sum of these two terms. So, that is what gives me these two terms over here. So, this e to the ikr is coming straight of this term and from this gamma times this logarithm I have these two terms which are coming from this is one source which comes here logarithm of twice kr right.

Sorry this is logarithm of twice kr which comes here and the other term is there is a gamma multiplying outside here so this gamma multiplies this twice logarithm sine theta by 2 which is coming here okay. So, these are the three terms now that we will track okay. (Refer Slide Time: 38:28)

$$\psi(\vec{r}) \rightarrow e^{i[\vec{k} \cdot \vec{r} - \gamma \ln(kr - \vec{k} \cdot \vec{r})]} + \tilde{f}_c(k, \theta) \frac{e^{i\left\{kr + \gamma \ln(2kr) + 2\gamma \ln \sin \frac{\theta}{2}\right\}}}{k(r-z)}$$

This result is often written as:

Eg. Eq.7.13.14 [p.437/Sakurai/MQM]

$$\psi(\vec{r}) \rightarrow e^{i[\vec{k} \cdot \vec{r} - \gamma \ln(kr - \vec{k} \cdot \vec{r})]} + f_c(k, \theta) \frac{e^{ikr} e^{i\gamma \ln(2kr)}}{k(r-z)}$$

$$f_c(k, \theta) = \tilde{f}_c(k, \theta) e^{i2\gamma \ln \sin \frac{\theta}{2}} = \left[\frac{\gamma}{2k \sin^2 \frac{\theta}{2}} \right] e^{i2\gamma \ln \sin \frac{\theta}{2}} e^{i\Theta(\gamma)}$$

NPTEL

PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2

89

Okay so, this is our solution now. And like I said Sakura he writes this with f_c rather than f_c tilda but then he has got a different phase here. So, the difference is absorbed in the phase factor but other than that there is no difference okay. So, it is essentially what you will find in Sakurai's book. So, this is the relationship which connects our notation f_c tilda with Sakurai's notation f_c .

So, this is the corresponding equivalence of which this is the common term and \tilde{f} is then what you find in this rectangular box times this difference which appears as a phase factor which is the upper case theta. So, this is also I have used a theta but this is not the polar coordinate theta this is the different one this is the upper case theta or the capital theta if I may call it. I am sure it has got a name of its own but Greek is not my language.

So, let me not worry about it. So, now to get the scattering amplitude that is the main interest in collision physics right. What is this scattering amplitude we know that its modulus square gives us the differential cross section when we integrate it over all the angles we will get the total scattering cross section.

So, that is essential interest in collision physics, so we want to find out what this whole thing in this rectangular box which goes in to \tilde{f} which is coming here what is it so that is our question.

(Refer Slide Time: 40:11)

$$\left[u \frac{d^2}{du^2} + (1-u) \frac{d}{du} - i\gamma \right] \chi(u) = 0 \quad u = ikv = ik(r-z)$$

The only singularity of this differential equation is at $u=0$; i.e. when $r = z$; $\cos\theta=1$; $\theta=0$ (i.e. along the polar axis)

Our solution must be regular at $u=0$.

$$\chi(u) = \int_{t_1}^{t_2} e^{ut} f(t) dt$$

t -space: Laplace transform space

NPTEL

PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 90

So, let us go back to the differential equation for you and now we have to worry about those singularities of this differential equation. So, where are the singularities there is only one and this is at $u = 0$ right. Because you are multiplying this d^2 over du^2 , so this is the only singularity of this and when is $u=0$, when $r = z$ because you are ik times $r - z$. And when is $r = z$ that is when $\theta = 0$ okay.

That is along the polar axis, so that is the only singularity. But then we want a solution which will be regular at $u = 0$. So, we will figure out how to get that, so what we will do is to make use of Laplace transforms and then use contour integration to evaluate these integrals. So, first we express the function χ in terms of the Laplace transform in the t space okay.

And this is our expression now and we have to find what will be the appropriate path of integration which will be acceptable to give us a physical solution for the Coulomb problem right. So, we have to find an appropriate path of integration in the complex t plane. So, you have got a complex t plane you have got the real axis and the imaginary axis. And the path of integration in the t plane is something that we have to determine. So, that we get physically acceptable solution.

(Refer Slide Time: 41:51)

$$\left[u \frac{d^2}{du^2} + (1-u) \frac{d}{du} - i\gamma \right] \chi(u) = 0 \quad \chi(u) = \int_{t_1}^{t_2} e^{ut} f(t) dt$$

$$\left[u \frac{d^2}{du^2} + (1-u) \frac{d}{du} - i\gamma \right] \int_{t_1}^{t_2} e^{ut} f(t) dt = 0$$

$$\int_{t_1}^{t_2} f(t) \left[u \frac{d^2 e^{ut}}{du^2} + (1-u) \frac{d e^{ut}}{du} - i\gamma e^{ut} \right] dt = 0$$

$$\int_{t_1}^{t_2} f(t) [ut^2 + (1-u)t - i\gamma] e^{ut} dt = 0$$

$$\int_{t_1}^{t_2} [(t - i\gamma) + t(t-1)u] e^{ut} f(t) dt = 0$$

PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 91

So, let us do that and this is your Laplace transform expression for the solution Chi okay. Now Chi is expressed as this integral, so I write this integral in place of this Chi over here okay. The differentiation is with respect to u integration is with respect to t okay. These are completely independent processes okay.

And I can write this differential equation this is actually an integro differential equation if you like it has got an integration part and there is a differential part. So, I can rewrite this equation as nothing is changed only that I have taken advantage of the fact that the integration with respect to t. So, it has got what are the integrands you have got the e to the ut. But these are operated upon by these differential operators.

Because the differentiation is with respect to u, so, e to the ut stays to the right of the differential operators okay, f of t can move to the left of the differential operators because differentiation is with respect to u. So, I have got integral t1 to t2 f of t. And then I have got a differential equation for u and integration with respect to the variable t okay, so here we are. So, let us write this.

Now I think we all know how to differentiate e to the ut with respect to u that is all there is to it okay. You take the first derivative take the second derivative, so you get ut square over here. You get 1 - u times t over here and then -i gamma e to the ut, u factor out okay. So, these are fairly straightforward manipulations and then you combine the terms. So, you get t - i gamma over here and then you get a term in u.

So, now this is the integru differential equation integration with respect to time and differentiation with respect to u has now been carried out. So, there is no further differentiation with respect to u that is left for us to worry about. The only thing we now have to do is to carry out the integration in the complexity plane choose a path of integration which is appropriate for the physical solution of the problem.

(Refer Slide Time: 44:30)

The slide contains the following mathematical content:

$$\int_{t_1}^{t_2} [(t-i\gamma) + t(t-1)u] e^{ut} f(t) dt = 0$$

$$\int_{t_1}^{t_2} \underbrace{t(t-1)f(t)u e^{ut}}_{1^{st} \text{ function}} dt + \int_{t_1}^{t_2} \underbrace{(t-i\gamma) e^{ut} f(t)}_{2^{nd} \text{ function}} dt = 0$$

$$\int_{x_1}^{x_2} f(x) \left\{ \frac{dg}{dx} \right\} dx = f(x)g(x) \Big|_{x_1}^{x_2} - \int_{x_1}^{x_2} \left\{ \frac{df}{dx} \right\} g(x) dx$$

Integral of the 2nd function $\rightarrow \int_{t_1}^{t_2} u e^{ut} dt = u \int_{t_1}^{t_2} e^{ut} dt = u \frac{e^{ut}}{u} \Big|_{t_1}^{t_2} = e^{ut} \Big|_{t_1}^{t_2}$

$$t(t-1)f(t)e^{ut} \Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \left\{ \frac{d}{dt} [t(t-1)f(t)] \right\} e^{ut} dt + \int_{t_1}^{t_2} (t-i\gamma) e^{ut} f(t) dt = 0$$

$$t(t-1)f(t)e^{ut} \Big|_{t_1}^{t_2} + \int_{t_1}^{t_2} \left\{ (t-i\gamma)f(t) - \frac{d}{dt} [t(t-1)f(t)] \right\} e^{ut} dt = 0$$

NPTEL logo is visible in the bottom left corner of the slide.

So, here you are, so this is the integral equation now okay. There is no more differentiation left. So, this is what you have got you have got two terms one coming from; you have got a t square and a t here. So, that is what gives you t square - t okay. So I have just read just said the terms and I would not spend much time commenting on these straightforward manipulations okay.

So, this integral now you solve as a product of two functions integral of a product of two functions. And that is a formula that we have it by heart from our high school day's right. So, you take this as your first function, this as the second function and then use this formula. You know the integral of the second because the integral of the second can be easily worked out which is ue to the ut.

And this is the difference you can take e to the ut at the upper limit 2t minus the value at the lower limit right. So, that is the integration that the result you get from the first term. And so

instead of this first term which is bracketed by this green beautiful bracket instead of this we have these terms. So, this is the difference term and now you have from the second term which is coming from here.

Actually from the usual formula of the integral of a product of two functions you do have a derivative with respect to time okay. So, this is one term that you get. And then there is another term which is under this blue bracket and that I have written as it is over here. So, now what we will do so this term comes here and these two terms I have rewritten here but I have moved this one to the left and this one to the right.

But it is essentially the same expression as in the previous step so there is no new physics nor new mathematics. But it is just it is going to give us a little convenient in handling or manipulating these terms. So, I have rewritten this solution so let me bring it to the top of the next slide.

(Refer Slide Time: 47:14)

$t(t-1)f(t)e^{ut} \Big|_{t_1}^{t_2} + \int_{t_1}^{t_2} \left\{ (t-i\gamma)f(t) - \frac{d}{dt} [t(t-1)f(t)] \right\} e^{ut} dt = 0$
 Assumption: surface terms vanish
 $\uparrow \text{Conditions?} \uparrow \quad \left\{ (t-i\gamma)f(t) - \frac{d}{dt} [t(t-1)f(t)] \right\} = 0$
 $(t-i\gamma)f(t) = \frac{d}{dt} [t(t-1)f(t)]$
 $\Rightarrow f(t) = At^{i\gamma-1}(1-t)^{-i\gamma}$
 Laplace
 $\chi(u) = \int_{t_1}^{t_2} e^{ut} f(t) dt$
 $\chi(u) = A \int_{t_1}^{t_2} e^{ut} t^{i\gamma-1} (1-t)^{-i\gamma} dt$
 $= A \int_{t_1}^{t_2} e^{ut} t^{i\gamma-1} (1-t)^{-i\gamma} dt$

Now so here it is exactly the same thing no further analysis done okay. And now suppose we make an assumption that the surface terms vanish that v's terms vanish if e to the ut vanishes at the extreme limits because you have to take the difference at the upper limit t2 and subtract from it the value at the lower limit t1, so these are the endpoints okay. And the endpoint is what I refer to as the points on the surface okay that is where the space ends.

So, far as our mathematical integration is concerned okay, so at these limits if we now assume why should I assume that why not if I can justify that assumption some way yes it is perfectly acceptable right. So, if we make this assumption and then we will going to we will ask of ourselves under what conditions can be assumed that the surface terms can be neglected okay.

So, if we presume that the surface terms vanish are we able to question ourselves and ask what are the conditions under, which the surface terms vanish? Then you do not have to worry about this okay. And in anticipation of a justification for that if we throw this term okay. We are going to have to find that justification we will find it.

And in anticipation of that if you forget about it then you need the integral t_1 to t_2 of this beautiful bracket times e to the ut dt should go to 0. And that will certainly be acceptable if what is in this beautiful bracket $t - i$ gamma times $f_t - d$ over dt and this term goes to 0 right. Because then the integral would vanish.

And then the mathematical form of the equation is nicely balanced subject to the consideration or subject to the justification that the surface terms would vanish. So, we will justify that and in the meantime let us continue to analyze this term here. So, what does this term give us it means this is the difference of two terms.

So, one term must be equal to the other term okay. So, this is $t - i$ gamma is equal to this and this is the first order derivative you can integrate it and get what f_t is. So, again I will not work out those details but you will get f_t to be given by some function of t which is just a single integration that is involved okay.

So, here you have got f_t given by this and now you can put this f_t in the Laplace expression okay because we have found out what this f_t should be. And then we will have to choose the path of integration in the complexity plane. Such that we can justify our assumption that the surface terms vanish okay that is the trick.

So, now this is the integral to be carried out in the complex t plane the contour C the path of integration from t_1 to t_2 is to be chosen appropriately.
(Refer Slide Time: 50:56)

$$t(t-1)f(t)e^{ut} \Big|_{t_1}^{t_2} + \int_{t_1}^{t_2} \left\{ (t-iy)f(t) - \frac{d}{dt} [t(t-1)f(t)] \right\} e^{ut} dt = 0$$

$$\chi(u) = A \int_{t_1}^{t_2} e^{ut} t^{iy-1} (1-t)^{-iy} dt$$

$$= A \int_{t_1}^{t_2} e^{ut} t^{iy-1} (1-t)^{-iy} dt$$

assumption
surface terms vanish

$$\int_{\text{Contour } C \text{ to be chosen}}$$

The diagram shows the complex t plane with the real axis ($\text{Re } t$) and imaginary axis ($\text{Im } t$). Two branch points are marked at $t=0$ and $t=1$ on the real axis. A branch cut is shown as a green line segment between $t=0$ and $t=1$. A blue rectangular contour C is drawn around the branch cut, with arrows indicating a clockwise direction. The contour is labeled as a 'rubber band distorted' branch cut. A small box indicates 'Contour C to be chosen'.

PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 94

So, this is what we have to solve this is the integral we have to solve. And the path is to be so chosen that the surface terms would vanish. So, this is the complex t plane and now we must observe that this is the integral that you have your solving and if you look at the integrand you know that there are these branch points at $t = 0$ and $t = 1$ okay. And then if you go around this then you can get multiple valued functions and so on.

So, if you want to avoid that you have to give a cut between the two. So, you can get a branch cut or you can distort the branch cutter right because you can this is what I think Sakurai has got a nice term for it is it an Sakurai's book or Landau Lifshitz book I forget. But one of them calls it as a rubber band distorted branch cut.

As if because you can flex it any which way and you can give a branch cut by stretching it in a manner that is convenient to you. So, this is the integral that you have to solve and you have to address the branch points appropriately.

(Refer Slide Time: 52:22)

$$t(t-1)f(t)e^{ut} \Big|_{t_1}^{t_2} + \int_{t_1}^{t_2} \left\{ (t-iy)f(t) - \frac{d}{dt} [t(t-1)f(t)] \right\} e^{ut} dt = 0$$

$$\chi(u) = A \int_{\text{Contour C to be chosen}} e^{ut} t^{iy-1} (1-t)^{-iy} dt$$

How should the path of integration be chosen?

Assumption: surface terms vanish


$u = ikw = ik(r-z)$

Asymptotic limit: $u \rightarrow \infty$ $u = ikr(1 - \cos \theta)$

$u = i\kappa$; with $\kappa \geq 0$ since $\cos \theta \leq 1$

Thus, to get $e^{ut} = e^{i\kappa t} \rightarrow 0$ we must have $t \rightarrow +i\infty$

These conditions determine the path of integration in the complex t-plane.



PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 95

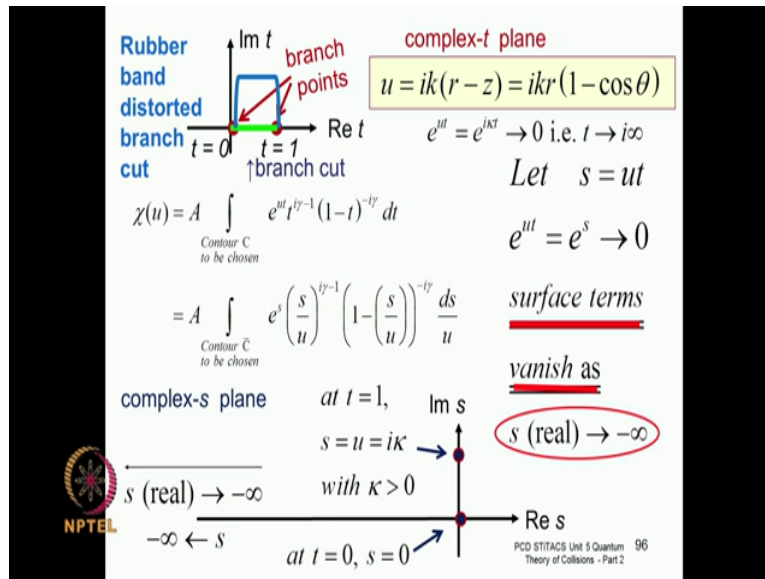
So, let us figure out how to do that. So, this is the problem now of which the surface terms we do not have to worry about. Except that we should keep at the back of our mind that we have made an assumption that the surface terms would vanish. And whatever control we choose now in the complexity plane must be such that the surface terms would vanish okay.

So that is the connection between the assumption that we make and the choice of the contour we will make in the complexity plane. So, now we have to choose the path of integration appropriately. So, that we can justify this assumption and again our solution our interest is in the asymptotic limit.

So our focus will be in the region u tending to infinity. Now let us look at this u what is u , u is $ikr - z$ or ikw and cosine theta is always less than or equal to 1. So, I can write this u as i times kappa where kappa is always greater than or equal to 0 okay. So, no matter what part of the space I am looking at Kappa will always be greater than or equal to 0. So now I want to get this e to the ut to go to 0 okay.

Because I want to kill the surface terms, so to kill the surface terms I require e to the ut to go to 0 and what is ut , ut is i times kappa times t and this should go to 0 and this will happen as t goes to minus infinity. So that tells me you know the path of integration how t can go to the positive infinity along the real image along the imaginary axis okay you have got the imaginary axis.

So, $+i$ infinity will make sure that our surface terms are destroyed okay that is the assumption we are making. So, these this is the condition which will have to be observed.
(Refer Slide Time: 54:52)



Now we can do this in the complex t plane subject to the discussion we just had. These are the branch points and you have the branch cut between them you have the rubber band distorted branch cut. But what we will do and here again I find Sakurai's treatment very attractive instead of carrying out the integration is a complex steeply and he carries out the integration in the complex s plane.

So, he defines s as u times t okay, so this is a simple transformation from t from u , from u , you define u into t as s . And now you want e to the ut to go to 0 right for the terms to go to zero and this means that s should go to minus infinity where it will be a real number. So, if you carry out the integration in the complex s plane instead of the complex t plane.

You now have the requirement to satisfy our assumption that we made that the surface terms vanish that s should go to minus infinity along the negative real axis in the complex s plane. So s will have to go to minus infinity, so let us write this integration not over t but over s . So, we carry out the integration in the complex s plane so instead of integrating over the variable t we are now integrating over s .

So, dt becomes ds over u t becomes s over you and so on. So, it is the same integrand I have effectively written okay. And now we have to choose a path of integration in the complex s plane. So, s must go to minus infinity along the negative real axis where are our branch points the branch point was at $t=0$ and $t=1$. And at $t=0$, s is 0 and at $t=1$ what is s , s is $i\kappa$.

So, $i\kappa$ is κ distance right above the first branch point but along the imaginary axis along the positive imaginary axis. So now these are your branch points you have a branch cut you have a rubber band distorted branch cut and you have to choose your path of integration to address these branch points appropriately.

(Refer Slide Time: 57:39)

complex-s plane

\bar{C}

$s = u$

$s = 0$

$u = ikr(1 - \cos \theta)$
 $= ik\kappa ; \kappa > 0$

$s = ut$

$e^{ut} = e^s \rightarrow 0$

$\chi(u) = A \int_{\bar{C}} e^s \left(\frac{s}{u}\right)^{\nu-1} \left(1 - \left(\frac{s}{u}\right)\right)^{-\nu} \frac{ds}{u} = A \int_{\bar{C}} e^s s^{\nu-1} (u-s)^{-\nu} ds$

Contour \bar{C} to be chosen

$\int_{\bar{C}} \equiv \int_{C_1} + \int_{C_2}$

consider the ratio: $\left(\frac{s}{u}\right)$

Asymptotic limit: $u \rightarrow \infty$

NPTEL PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 97

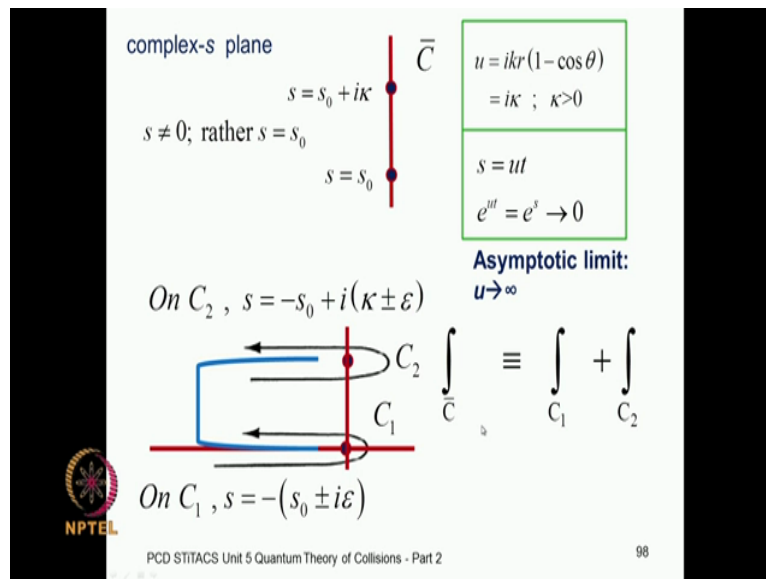
So, this is our Chi function written as an integral. So, this is nothing but the Laplace expression that we add and it is now written as an integral over s. Now this is again simple manipulation you have got a 1 over u to the power -1 but then you have got a 1 over u here okay. So, when you take care of these terms you get a rather simple form.

Which is completely equivalent there is nothing new in the extreme expression here compared to this it is exactly the same thing okay. So, now you have to choose a contour appropriately okay, so how would you do that. So, we know that you can choose this contour C bar which is the contour over which we have to carry out this integration. We can do it over a sum of two contours one going around the first branch point.

And the other going around the second branch point because the point at infinity is just the point at infinity in the complex plane okay. So, let it go all the way to the infinite distance along the real x axis in the negative direction. So, these are the two contours that we will choose. So, we will take the sum of C integrals over the contours C1 and C2.

So, these are the two contours C1 is this and the C2 is this. And let us consider the ratio s over u because we are also focusing on the asymptotic limit u going to infinity right. So, we can develop an expansion in s over u. So, you consider the ratio s over u,

(Refer Slide Time: 59:42)



So, let us go to the next slide. And what is going to happen is that as t changes or u changes s will change right. And in the previous figure we had $s = 0$ over here. But then if you can have some other values because s is after all a product of u and t okay. So, it may have some of the values.

So, when it has some other value let us say it has got a typical value like s_0 , s_0 is one of those values it does not matter what. Then the corresponding branch points will be at s_0 plus the second branch point will be $i\kappa$ times or i kappa times above it on a line which is parallel to the imaginary axis okay.

So, that will be the second branch point. So, you can get to the real axis itself from this s_0 if you subtract this s_0 okay. Then all this contour C_1 the value of s will be $-s_0$ because you will have to subtract that to get to the real axis. And then you will have to add or subtract a little bit distance orthogonal to the real axis which will be i epsilon okay.

Because the control will be as close infinitesimally close to the real axis just at epsilon distance above it and epsilon below that so you on the contours C_1 , s will be minus of s_0 plus or minus i epsilon. And over C_2 it will be the same but you will have to add i kappa to that.

So, here it is the same but you have added i kappa on the curve C_2 okay. So, these are the two integrals that we now have to determine. So, on C_2 we displayed what will be the values of s but what is our interest, our interest is in the asymptotic region. So, we will be developing expansions or approximations in s over u . So, let us find out what happens to s over u okay.

(Refer Slide Time: 1:02:11)

$s = s_0 + i\kappa$
 $s = s_0$

$u = ikr(1 - \cos \theta)$
 $= i\kappa ; \kappa > 0$

$u \rightarrow \infty ; \kappa \rightarrow \infty \quad \frac{s}{u} \rightarrow \text{small on } C_1$
 $\frac{s}{u} \rightarrow \text{not small on } C_2$

Asymptotic limit:

complex-s plane
 On C_2 , $\frac{s}{u} = \frac{-s_0 + i(\kappa \pm \epsilon)}{i\kappa} = 1 - \frac{s_0 \mp i\epsilon}{i\kappa}$
 On C_1 , $\frac{s}{u} = -\frac{(s_0 \pm i\epsilon)}{i\kappa}$

$\int_{\bar{C}} \equiv \int_{C_1} + \int_{C_2}$

ITACS Unit 5 Quantum Theory of Collisions - Part 2 99

So, this is the choice of the contours and the corresponding values of s over u will be the value of s divided by the value of u which is $i \kappa$ as we know right. So, s over u will be simply the value of s on C_1 it will be $s_0 +$ or $- i \epsilon$ divided by $i \kappa$ and on C_2 you will have to add that $i \kappa$ right.
 (Refer Slide Time: 1:02:43)

$\chi(u) = A \int_{\text{Contour } C} e^s \left(\frac{s}{u}\right)^{iy-1} \left(\frac{u-s}{u}\right)^{-iy} \frac{ds}{u}$

$u = ikr(1 - \cos \theta)$
 $= i\kappa ; \kappa > 0$

On C_1 , $\frac{s}{u} = -\frac{(s_0 \pm i\epsilon)}{i\kappa}$ On C_2 , $\frac{s}{u} = \frac{-s_0 + i(\kappa \pm \epsilon)}{i\kappa} = 1 - \frac{s_0 \mp i\epsilon}{i\kappa}$

Asymptotic limit: $u \rightarrow \infty ; \kappa \rightarrow \infty$

$\frac{s}{u} \rightarrow \text{small on } C_1$; $\frac{s}{u} \rightarrow \text{not small on } C_2$

To develop an approximation in which we may ignore higher powers of $\left(\frac{s}{u}\right)$, $(u-s)$ can be expanded in powers of $\left(\frac{s}{u}\right)$ on C_1 , but not on C_2 .

PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 100

So, this is the value on C_1 and on C_2 when you add this $i \kappa$ over here what do you get. Now do this a little carefully now, this $i \kappa$ when divided this $i \kappa$ gives you 1 okay and then you have this $-s_0$ and then $-$ or $+$ of $i \epsilon$. Whereas on C_1 s over u is given by this ratio, so there is a little difference between the two because on C_1 as u tends to infinity or as competence to infinity okay s over u can be neglected.

Because you have got combined the denominator but on C_2 , κ is in the denominator in the second term but here you have got 1, so you really have to be careful here okay. So, s over u is small on C_1 and in the asymptotic limit you will be able to throw s over u . But you

cannot do so on the curve C2 okay C2 is the one which was above the C1 by a factor of i times kappa right.

So now to develop an approximation in which we can ignore higher powers of s over u. We cannot expand it in terms of s over u and throw those terms on curve C2, so that is the point that we have to worry about.
(Refer Slide Time: 1:04:30)

On C_2 , $\frac{s}{u} = \frac{-s_0 + i(\kappa \pm \varepsilon)}{i\kappa} = 1 - \frac{s_0 \mp i\varepsilon}{i\kappa}$ change the variable $s \rightarrow s' = s - u$

On C_2 , $\frac{s}{u} = \frac{s' + u}{u}$ $\left| \frac{s'}{u} = \frac{s - u}{u} = \frac{s}{u} - 1 = 1 - \frac{s_0 \mp i\varepsilon}{i\kappa} - 1 = -\frac{s_0 \mp i\varepsilon}{i\kappa} \right|$

Asymptotic limit: $u \rightarrow \infty$; $\kappa \rightarrow \infty$

$\frac{s}{u} \rightarrow \text{small on } C_1$; $\frac{s}{u} \rightarrow \text{not small on } C_2$; $\frac{s'}{u} \rightarrow \text{small on } C_2$

$\int_C \equiv \int_{C_1} \frac{ds}{u} + \int_{C_2} \frac{ds}{u}$

$\equiv \int_{C_1} \frac{ds}{u} + \int_{C_1} \frac{ds'}{u}$

$s = s' + u$
 $s' = s - u$

NPTEL
PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2
Sakurai / Eq.7.13.22 (page 438) 101

So, again we use one transformation the manipulations are very simple but they are very interesting. So, you carry out another transformation you now change the variable instead of s you go to s prime. And you define s prime by s - u what will s prime do s prime will bring all points over here on the contour C2 as a point goes along the path on C2 and at each point if you subtract i kappa you will be going over C1 right.

So, you can transform the integral from C2 to C1 by changing the integration variable from s to s prime. So let us do that, so that is the main thing rest of it is manipulation which is quite simple. But let us see how it works out, so on C2 you have s over u, s is now defined as s prime is s - u, so s will be s prime + u right.

So, you have s prime + u over u on the curve C2. And now if you ask yourself what is s prime over u let s prime over u is this factor and in the asymptotic limit you can throw it just as you did the s over u for the curve C1 okay. So, you have got a similar kind of situation resulting.

But the difference is that you have to subtract this i kappa from every point okay. So, you now have s over u which will be ignorable in the asymptotic limit on C1, s prime over u ignorable C2. But s over u itself is not small on C2 okay. So, now you can transform the

integration which is over s to integration over s prime but then carry out the integration over C1 because you have subtracted that i kappa from every value of s okay.

So, now this is the, these are the two integrals we now have to determine now rest of it is again very straight forward integration there is absolutely nothing in it. So, I will not spend any not much time doing that but I will show you some of the main features of that.
(Refer Slide Time: 1:07:12)

$$\chi(u) = A \int_{\text{Contour } \bar{C} \text{ to be chosen}} e^s \left(\frac{s}{u}\right)^{\gamma-1} \left(1 - \left(\frac{s}{u}\right)\right)^{-\gamma} \frac{ds}{u}$$

$$\chi(u) = A \left\{ \int_{C_1} e^s \left(\frac{s}{u}\right)^{\gamma-1} \left(\frac{u-s}{u}\right)^{-\gamma} \frac{ds}{u} + \int_{C_1} e^{s'+u} \left(\frac{s'+u}{u}\right)^{\gamma-1} \left(\frac{u-s'-u}{u}\right)^{-\gamma} \frac{ds'}{u} \right\}$$

$s' = s - u$


$$\chi(u) = A \left\{ \int_{C_1} e^s s^{\gamma-1} (u-s)^{-\gamma} ds \right\} + \left\{ \int_{C_1} e^{s'+u} (s'+u)^{\gamma-1} (-s')^{-\gamma} ds' \right\}$$

PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 102

So, now you have got s prime is s - u the integration is now to be carried out in the first term over C1, over the variable s. But over this the second integral is now to be carried out again over the same contour C1 but not over s but over s prime. So, I have written the second integration in terms of s prime.

So that the integrands are expressed in terms of s prime, rest of it is just substituting equivalent terms nothing else okay. So, it is very simple and I will not spend any time demonstrating these substitutions they are all there over you okay. So, here you are so you have these two integrations one is over C1 the other is also over C1 but over the variable s prime rather than s.

(Refer Slide Time: 1:08:16)



$$\chi(u) = A \left\{ \left[\int_{C_1} e^s s^{\gamma-1} (u-s)^{-\gamma} ds \right] + \left[\int_{C_1} e^{s+u} (s'+u)^{\gamma-1} (-s')^{-\gamma} ds' \right] \right\} \quad C_2: \quad s \rightarrow s' = s - u$$

$$\chi(u) = A \left\{ \left[\int_{C_1} e^s s^{\gamma-1} \left(u \left(1 - \frac{s}{u} \right) \right)^{-\gamma} ds \right] + \left[\int_{C_1} e^{s+u} \left(u \left(1 + \frac{s'}{u} \right) \right)^{\gamma-1} (-s')^{-\gamma} ds' \right] \right\}$$


$$\chi(u) = A \left\{ \left[\int_{C_1} e^s s^{\gamma-1} u^{-\gamma} \left(1 - \frac{s}{u} \right)^{-\gamma} ds \right] + \left[\int_{C_1} e^{s+u} u^{\gamma-1} \left(1 + \frac{s'}{u} \right)^{\gamma-1} (-s')^{-\gamma} ds' \right] \right\}$$

PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 103

So, now we bring it to the top of this slide over here. Now what have I done here nothing very much again you have got $u - s$ to the power $-i$ gamma, so I factor u , so you have u into $1 - s$ over u the whole thing to the power $-i$ gamma okay. So, just because some of these mathematical terms look big on the screen does not mean that they are complicated they are not okay.

It is just simple substitution I have done the same thing in the second term for obvious reasons that we want to develop an expansion in s over u or s prime over u right. So, these are the two terms and now you have a u to the power $-i$ gamma which is written here. And then you have got $1 - s$ over u to the power $-i$ gamma which is written here. I have done a similar thing in the second term okay.

So, let us take this and then our interest will be in developing expansions and powers of s over u or s prime over u both on the contours C_1 .
(Refer Slide Time: 1:09:29)



$$\chi(u) = A \left\{ \begin{aligned} & \left[\int_{C_1} e^s s^{i\gamma-1} u^{-i\gamma} \left(1 - \frac{s}{u}\right)^{-i\gamma} ds \right] + \\ & \left[\int_{C_1} e^{s+u} u^{i\gamma-1} \left(1 + \frac{s'}{u}\right)^{i\gamma-1} (-s')^{-i\gamma} ds' \right] \end{aligned} \right\}$$


Use < s (dummy) > in both the integrals:

$$\chi(u) = A \left\{ \begin{aligned} & u^{-i\gamma} \left[\int_{C_1} e^s s^{i\gamma-1} \left(1 - \frac{s}{u}\right)^{-i\gamma} ds \right] + \\ & u^{i\gamma-1} e^u (-1)^{-i\gamma} \left[\int_{C_1} e^s \left(1 + \frac{s}{u}\right)^{i\gamma-1} s^{-i\gamma} ds \right] \end{aligned} \right\}$$

PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 104

So, these are the two integrals and now in the second integral s prime is a dummy anyway. So, I can call it anything else I can call it z or x or y or why not s itself okay. What is in a name right, so I am going to call it as s just for convenience okay? Also sometimes to confuse you and make sure that you are not sleeping okay but it is the same.

So it is exactly the same integral because it is just a dummy integration label its gets integrated out. So, this is; these are the two integrals now alright.
(Refer Slide Time: 1:10:16)



$$\chi(u) = A \left\{ \begin{aligned} & u^{-i\gamma} \left[\int_{C_1} e^s s^{i\gamma-1} \left(1 - \frac{s}{u}\right)^{-i\gamma} ds \right] + \\ & u^{i\gamma-1} e^u (-1)^{-i\gamma} \left[\int_{C_1} e^s \left(1 + \frac{s}{u}\right)^{i\gamma-1} s^{-i\gamma} ds \right] \end{aligned} \right\}$$

7.13.24
p.440
Sakurai
Modern
Quantum
Mechanics

Asymptotic limit:

$$u \rightarrow \infty$$

$$\chi(u) \approx A \left\{ \begin{aligned} & u^{-i\gamma} \left[\int_{C_1} e^s s^{i\gamma-1} ds \right] + \\ & u^{i\gamma-1} e^u (-1)^{-i\gamma+1} (-1) \left[\int_{C_1} e^s s^{-i\gamma} ds \right] \end{aligned} \right\}$$

$\left(\frac{s}{u}\right) \rightarrow 0$


$$\chi(u) \approx A \left\{ \begin{aligned} & \left[u^{-i\gamma} \int_{C_1} e^s s^{i\gamma-1} ds \right] - \left[e^u (-u)^{i\gamma-1} \int_{C_1} e^s s^{-i\gamma} ds \right] \end{aligned} \right\}$$

PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 105

So, now we are interested in the asymptotic limit and in the asymptotic limit you can throw the s over u okay. So, in the asymptotic limit you throw the s over u and then the rest of the terms for this asymptotic limit when s over u goes to 0 or u goes to infinity you have relatively simpler integrals now okay. We have already chosen the contours and I write these two terms in over here. So, what have we got here we have got this e to the u -u to the power i gamma - 1 and then you have got this

integral here okay. So it is just rearrangement of the terms and again nothing fancy about this okay.

(Refer Slide Time: 1:11:19)



$$\chi(u) \approx A \left\{ \left[u^{-i\gamma} \int_{C_1} e^s s^{i\gamma-1} ds \right] - \left[e^u (-u)^{i\gamma-1} \int_{C_1} e^s s^{-i\gamma} ds \right] \right\}$$

$$\chi(u) = 2\pi i A \left\{ u^{-i\gamma} g_1(\gamma) - (-u)^{i\gamma-1} e^u g_2(\gamma) \right\}$$

$$2\pi i g_1(\gamma) = \int_{C_1} e^s s^{i\gamma-1} ds \quad ; \quad 2\pi i g_2(\gamma) = \int_{C_1} e^s s^{-i\gamma} ds$$

$$2\pi i g_2(\gamma) = \int_{C_1} s^{-i\gamma} e^s ds = s^{-i\gamma} e^s \Big|_{-x-i\epsilon}^{-x+i\epsilon} - \int_{C_1} (-i\gamma) s^{-i\gamma-1} e^s ds$$

$$= (i\gamma) \int_{C_1} s^{-i\gamma-1} e^s ds = (i\gamma) g_1^*(\gamma) 2\pi i$$


PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 106

So, here you are and what we do to get a solution in a compact form and something that we can really discuss easily introduce these functions g_1 and g_2 where these are defined as twice $\pi i g_1$ is defined by this integral. So, instead of this integral I could use twice $\pi i g_1$ okay. And likewise I can use twice $\pi i g_2$ over here. So, this is just defining some new terms which are completely equivalent to what we are already doing.

And there is no major transformation or anything which is involved it is just substituting the terms that we already have in terms of new symbols a new notation which is defined in terms of the old notation. So, this is just a change of notation and nothing else. So, you now have these two instead of these two integrals you have the g_1 and the g_2 okay instead of the two integrals.

So, you can see that one of them is can be written in terms of the complex conjugate of the other by a little bit of substitution.

(Refer Slide Time: 1:12:46)



$$\chi(u) = 2\pi i A \left\{ u^{-i\gamma} g_1(\gamma) - (-u)^{i\gamma-1} e^u g_2(\gamma) \right\}$$

$$2\pi i g_1(\gamma) = \int_{C_1} e^s s^{i\gamma-1} ds ; 2\pi i g_2(\gamma) = \int_{C_1} e^s s^{-i\gamma} ds$$


$$2\pi i g_2(\gamma) = (i\gamma) \int_{C_1} s^{-i\gamma-1} e^s ds = (i\gamma) g_1^*(\gamma) 2\pi i \quad \begin{matrix} u = ikr(1 - \cos\theta) \\ = ikr ; k > 0 \end{matrix}$$

$$\begin{aligned} \chi(u) &= 2\pi i A \left\{ u^{-i\gamma} g_1(\gamma) - (-u)^{i\gamma-1} e^u (i\gamma) g_1^*(\gamma) \right\} \\ &= 2\pi i A \left\{ u^{-i\gamma} g_1(\gamma) - (u^*)^{i\gamma-1} e^u (i\gamma) g_1^*(\gamma) \right\} \\ &= 2\pi i A u^{-i\gamma} g_1(\gamma) \left\{ 1 - (u^*)^{i\gamma} (u^*)^{-1} e^u \frac{1}{u^{-i\gamma} g_1(\gamma)} (i\gamma) g_1^*(\gamma) \right\} \end{aligned}$$

PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 107

And now you have the g_1 and g_2 over here these are the two integrals that we have already discussed. These are their explicit forms and what have we got now we have one the complete solution. Because the solution for χ is nothing but the sum of these two terms. So, you put those two terms here rearrange the terms and as you can see that there is nothing fancy which is being done here.

It is like u^* to the power $i\gamma - 1$ is written as u^* to the power $i\gamma$ multiplied by u^* to the power -1 okay nothing big okay. So, on the screen these equations look big whether they are very simple and straightforward okay.
(Refer Slide Time: 1:13:48)



$$\chi(u) = 2\pi i A u^{-i\gamma} g_1(\gamma) \left\{ 1 - (u^*)^{i\gamma} (u^*)^{-1} e^u \frac{1}{u^{-i\gamma} g_1(\gamma)} (i\gamma) g_1^*(\gamma) \right\}$$

$$\chi(u) = 2\pi i A u^{-i\gamma} g_1(\gamma) \left\{ 1 - \frac{(u^*)^{i\gamma} g_1^*(\gamma)}{u^{-i\gamma} g_1(\gamma)} (i\gamma) \frac{e^u}{(u^*)} \right\}$$

$$\chi(u) = 2\pi i A u^{-i\gamma} g_1(\gamma) \left\{ 1 + \frac{(u^*)^{i\gamma} g_1^*(\gamma)}{u^{-i\gamma} g_1(\gamma)} (i\gamma) \frac{e^u}{u} \right\}$$

$$\chi(u) = 2\pi i A u^{-i\gamma} g_1(\gamma) \left\{ 1 + e^{\phi(k,u,\gamma)} (i\gamma) \frac{e^u}{u} \right\}$$

where $e^{\phi(k,u,\gamma)} = \frac{(u^*)^{i\gamma} g_1^*(\gamma)}{u^{-i\gamma} g_1(\gamma)} = \frac{(u^{-i\gamma})^* g_1^*(\gamma)}{u^{-i\gamma} g_1(\gamma)} = \frac{[u^{-i\gamma} g_1(\gamma)]^*}{u^{-i\gamma} g_1(\gamma)}$

PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 108

So, now you have these terms here and you rearrange the terms a little bit you find out so you write this in the denominator put it here, you put this one on top of this. So, that it looks neater, so this is nothing but the same expression except that it takes less space to write it. It

is written in a more compact form that is all okay. And we continue this simple analysis or simple manipulation of these terms.

And now you write this in terms of a ratio of g_1 star over g_1 and this ratio of the u star and you and you write this ratio in terms of a phase factor because it is some complex number which you write as a phase e to the i Phi. So, e to the i Phi is nothing but this phase factor. Now this is just to finally get a form.

So, that what we have done using our notations most places we have stayed very close to the notation in Sakurai wherever we have departed. We have this additional phase which I have shown the upper case capital theta which I had introduced other that it is same. (Refer Slide Time: 1:15:15)

The slide contains the following mathematical derivations:

$$\chi(u) = 2\pi i A u^{-i\gamma} g_1(\gamma) \left\{ 1 + e^{i\phi(k,u,\gamma)} (i\gamma) \frac{e^u}{u} \right\} \text{ where } e^{i\phi(k,u,\gamma)} = \frac{[u^{-i\gamma} g_1(\gamma)]^*}{u^{-i\gamma} g_1(\gamma)}$$

$$u = ikr(1 - \cos\theta) = i\kappa ; \quad \kappa > 0$$

!Eq 7.13.27 * 7.13.28 p.440/Sakurai/MQM

$$(u)^{-i\gamma} = (i\kappa)^{-i\gamma} = (i)^{-i\gamma} [k(r-z)]^{-i\gamma} = e^{\frac{\gamma\pi}{2}} e^{-i\gamma \ln[k(r-z)]}$$

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \chi(u)$$

$$= e^{ikr \cos\theta} 2\pi i A e^{\frac{\gamma\pi}{2}} e^{-i\gamma \ln[k(r-z)]} g_1(\gamma) \left\{ 1 + e^{i\phi(k,u,\gamma)} (i\gamma) \frac{e^u}{u} \right\}$$

$$\psi(\vec{r}) = 2\pi i A e^{\frac{\gamma\pi}{2}} e^{i\{kz - \gamma \ln[k(r-z)]\}} g_1(\gamma) \left\{ 1 + e^{i\phi(k,u,\gamma)} (i\gamma) \frac{e^u}{u} \right\}$$

NPTEL PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 109

So, here you are, so this is u to the $-i$ gamma we are going to need it here. And in terms of this you can now write the solution which is e to the ikz times χ of u , χ of u is here. So, now we already have the full solution okay. We already have the full solution we have obtained it using the appropriate contour which will give us the physically acceptable solution. It we started out by proposing some solutions and then we argued that okay.

Those will be acceptable solutions subject to certain conditions and our there was various approximation that we discussed. But our primary concern was that we had to throw off the surface terms. And then we discussed how we can choose the contour in the complex s plane so that we can throw the end effects okay. So, that we can justify our choice and now we have the final solution.

We it is nice to rearrange it in a form which will be very familiar and the most exciting part of this analysis is that the end result is something that you could have got even without doing

quantum theory, so that is the interesting part. So, let me show you how you get that. So, here you have got the wave function and you have the full solution written in terms of this g_1 and the phase factor of Φ now.
 (Refer Slide Time: 1:16:55)

$$\psi(\vec{r}) = 2\pi i A e^{\frac{\gamma}{2}} g_1(\gamma) \left\{ e^{i(kz - \gamma \ln[k(r-z)])} + e^{i\theta(k,u,\gamma)} \frac{\gamma}{2k \sin^2 \frac{\theta}{2}} \frac{e^{i(kr - \gamma \ln[k(r-z)])}}{r} \right\}$$

$$\psi(\vec{r}) = 2\pi i A e^{\frac{\gamma}{2}} g_1(\gamma) \left\{ e^{i(kz - \gamma \ln[k(r-z)])} + \frac{\gamma}{2k \sin^2 \frac{\theta}{2}} \frac{(u^*)^\gamma}{u^{-\gamma}} \frac{g_1^*(\gamma)}{g_1(\gamma)} \frac{e^{i(kr - \gamma \ln[k(r-z)])}}{r} \right\}$$

$(u^*)^\gamma = e^{\frac{\gamma}{2}} e^{i\gamma \ln[k(r-z)]}$	$\frac{(u^*)^\gamma}{(u)^{-\gamma}} = e^{2i\gamma \ln[k(r-z)]}$	$\frac{g_1^*(\gamma)}{g_1(\gamma)} = e^{i\theta(\gamma)}$
---	---	---

$$\psi(\vec{r}) = 2\pi i A e^{\frac{\gamma}{2}} g_1(\gamma) \left\{ e^{i(kz - \gamma \ln[k(r-z)])} + \frac{\gamma}{2k \sin^2 \frac{\theta}{2}} e^{2i\gamma \ln[k(r-z)]} e^{i\theta(\gamma)} \frac{e^{i(kr - \gamma \ln[k(r-z)])}}{r} \right\}$$

$$\psi(\vec{r}) = 2\pi i A e^{\frac{\gamma}{2}} g_1(\gamma) \left\{ e^{i(kz - \gamma \ln[k(r-z)])} + \frac{\gamma}{2k \sin^2 \frac{\theta}{2}} e^{i\theta(\gamma)} \frac{e^{i(kr + \gamma \ln[k(r-z)])}}{r} \right\}$$

NPTEL
PCD STTACS Unit 5 Quantum Theory of Collisions - Part 2
Eq. 7.13.30
p.441/Sakurai/MQM
111

So, this is your phase okay. So, let us write these terms now and focus attention on the main part of the solution because whatever constants are there we would not worry about them okay. So, $2\pi i$ and A and so on that they must be there okay. So, do not get me wrong I am not saying that okay they are not important and you can mess them up because if you do that in an exam you end up getting a zero.

So, those terms are important but they are not important so far is the physics of the problem is concerned. So, you factor out all these terms and γ you remember is coming from the z_1, z_2 and the okay. The k was also sitting over there, so you have these factors here $r - z$ from geometry we knew goes as twice sine square theta by 2 we discussed that earlier okay. So, we will use that put this $r - z$ in terms of this factor here.

Because that enables us to write it in a form which we are going to find in Sakurai's book so here you have that. Again simple rearrangement of terms we know what is u^* to the power $i\gamma$ and u to the power $-i\gamma$. So, these have been written out explicitly over here. So, we can write this ratio also over here and this is the ratio which is e to the i uppercase theta okay.

So, this factor can be; so instead of writing it in terms of g_1 and g_1^* , we can now write the solution in terms of e to the i theta. And in terms of e to the i theta we find this solution to be given by this. So, this is pretty much the solution that you will find. So, we have got this

solution written in a form which has got and which looks like an incoming wave and spherically outgoing wave.

With the difference that the incoming wave has got a phase here which is r dependent? And the outgoing wave also has got a phase which is our dependent. So, you can really never separate the incoming wave from the outgoing wave in the Coulomb problem okay. It is because the interaction has got an infinite range okay. So, this is a very peculiar feature of the Coulomb problem.

(Refer Slide Time: 1:19:54)

$$\psi(\vec{r}) = 2\pi i A e^{i\frac{\pi}{2}} g_1(\gamma) \left\{ e^{i[kz - \gamma \ln k(r-z)]} + \frac{\gamma}{2k \sin^2 \frac{\theta}{2}} e^{i\theta(\gamma)} \frac{e^{i[kr + \gamma \ln k(r-z)]}}{r} \right\}$$

$$r-z = r - r \cos \theta = r(1 - \cos \theta) = r \left(2 \sin^2 \frac{\theta}{2} \right)$$

$$\psi(\vec{r}) \rightarrow e^{i[kz - \gamma \ln k(r-z)]} + f_c(k, \theta) \frac{e^{ikr} e^{i\gamma \ln(2kr)}}{k(r-z)}$$

$$f_c(k, \theta) = \frac{\gamma}{2k \sin^2 \frac{\theta}{2}} e^{i\left\{ \theta(\gamma) + 2\gamma \ln \sin \frac{\theta}{2} \right\}}$$

$$\frac{d\sigma}{d\theta} = |f_c(k, \theta)|^2 = \frac{\gamma^2}{4k^2 \sin^4 \frac{\theta}{2}}$$

Next unit:
RESONANCES

← Rutherford formula

Bye!

NPTEL QUESTIONS ? Write to: pcd@physics.iitm.ac.in
 PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2

So, you really cannot separate the incoming wave from the outgoing way but you can write it in a form which is corresponds to the standard solution in collision physics. And now we can write it in terms of the fc which is the Sakurai's fc whereas we had f tilde earlier. But the fc now absorbs this e to the i theta the upper case theta okay. And this is now what you would regard as the scattering amplitude.

Its modulus square will give you the differential cross section and what do you get for the differential cross section, what is this modulus square this is just a phase factor so this will drop off it does not matter right. It does not matter what do you get, you just get the classical result and you would say why did I have to do quantum theory okay. Now this is a very, very interesting feature of the Coulomb problem.

That the classical Rutherford formula then in our; was it in the first class of this unit or in the second I think the second we did the Born approximation for the Coulomb problem and we did it for the screen Coulomb right. So, we did the Yukawa potential and that gave us the same result.

So, the Yukawa potential, the Born approximation, the classical Rutherford and the quantum mechanical collision two center problem they all give the same result and these are some very peculiar features of the Coulomb problem and this is because of an exceptional symmetry that the $1/r$ potential has.

And we commented on this in our previous course on atomic physics that you have got this the S_4 symmetry which is a dynamical symmetry which comes from the $1/r$ strict nature of the potential, so the corresponding classical analog is the conservation of the Laplace Runge vector for the $1/r$ potential okay for the quantum-mechanical case it is the S_4 symmetry of the hydrogen atom.

And this of course breaks down for other items including atoms in the first group of the periodic table. So, although they have got similar valence shell structure they have very different you know physical properties sometimes and it is because they all depart from the $1/r$ like the sodium atom. So, what does it do to the $1/n^2$ for the discrete states it introduces the quantum defect okay?

So, instead of the $1/n^2$ you get a $1/(n - \mu)^2$. So, thank you very much we will conclude this unit over here and in the next unit we will discuss resonances we will get into the Breit Wigner and then the Fano Feshbach resonances in the next. So, we have four classes in unit 6 and another four in unit 7. So, we will be doing the resonances.