Select/Special Topics in Atomic Physics
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Lecture - 29
Probing the Atom
Collisions and Spectroscopy – Boundary Conditions
Time Reversal Conditions and its Applications in Atomic Collisions and Photoionization Processes

Today, we are going to conclude unit 6, and in this we are our focus is on recognizing the connections between the solution to the collision problem, and solution to the photo ionization problem. And I mentioned that these solutions are connected to each other by the time reversal symmetry, so today we will establish these connections conclusively.

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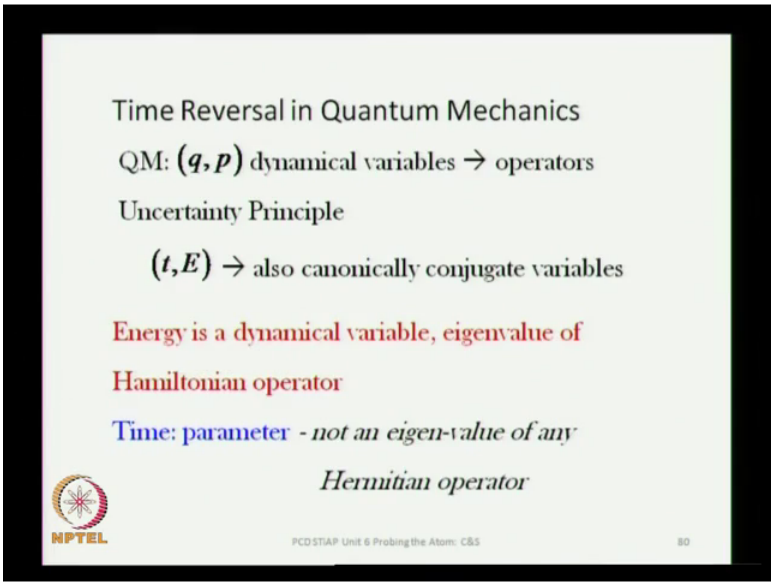

And we need to understand what is meant by time reversal symmetry in quantum mechanics, so I will not get into too many details about it, but I will certainly explain what is meant by time reversal in quantum mechanics. It is quite different from what it is the classical mechanics, which we discussed in our previous class. Now, to begin with we recognize that there is uncertainty between position and momentum, and this is the generalized position and the generalized momentum.

So, it can be anything it does not have to be the physical x position, and the physical linear momentum along the x direction. It can be any two canonically conjugate variables, which are generalized position and the momentum, which is canonically conjugate to that, and in this sense time and energy are also canonically conjugate. So, they also qualify for this, but the uncertainty principle for energy and time, it has a very different basis than what it is for position and momentum.

Although, there is a certain similarity, so there is this delta q delta p business, and likewise there is a delta t delta e business, the uncertainty between energy and time. But, the foundation of the uncertainty principle for energy and time is completely different from, what it is for position and momentum, the reason is that there is really no operator for time in quantum mechanics. Time is just a parameter in quantum mechanics, energy is a dynamical variable for which there is an operator, the operator for energy is the Hamiltonian operator, but there is no operator for time in quantum mechanics. So, the foundation of the uncertainty principle, for energy and time is quite different and that is important in recognizing, what is meant by time reversal symmetry, because there is no operator for time.

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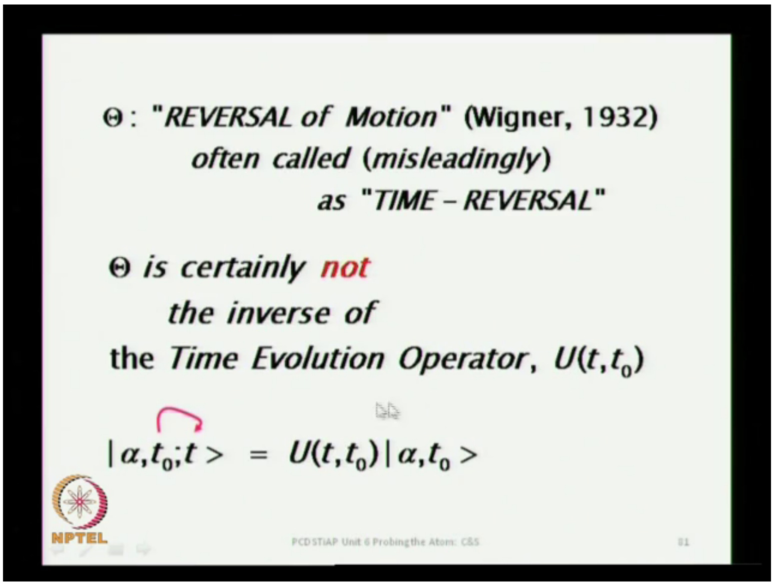

Now, it is just a variable it is a parameter which changes continuously, it is not an Eigen value of any operator and; that means, that what is meant by time reversal has to be understood, in its own context in quantum mechanics. This should be correctly be called as motion reversal, as Wigner suggested, but it is often referred to as time reversal, a little bit of misleading terminology, but it is quite common.

So, everybody uses it and we are going to use it, but we are going to remember, that what is actually being implied is motion reversal is more appropriate expression for what we are talking about than time reversal. This was introduced by Wigner in 1932, and time reversal is certainly not the inverse of time evolution, so that is the first thing that we will you know spell out. So, before we tell, before we discuss what time reversal is we will highlight what it is not.

So, it is not the inverse of time evolution operator, and let me remind what the time evolution operator does, so U is a time evolution operator, what it does is it operates on a state at time t 0. And from this it gives you the state at a later time t, so this is a time evolution operator, so it tells you how the system evolves from a time t 0 to t, so that is what is meant by time evolution.

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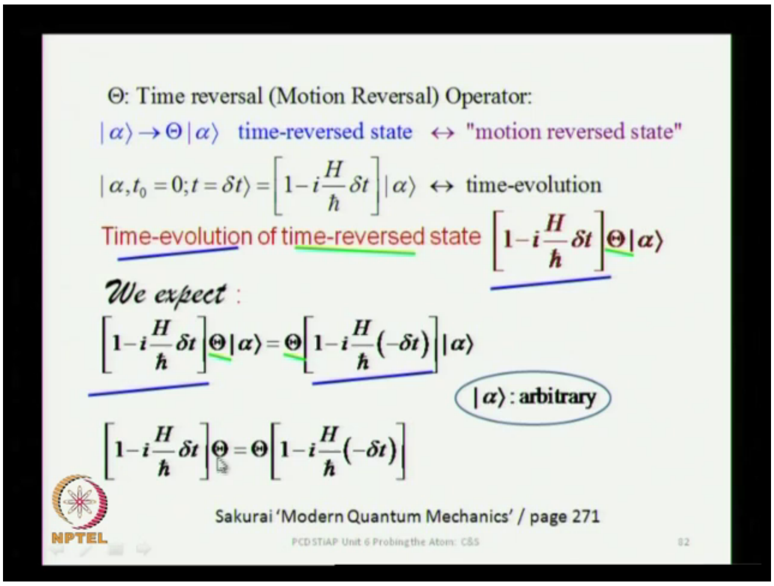

So, now, we will introduce time reversal or motion reversal, and this is what time evolution is that if alpha is in arbitrary state. We operate it on by the time evolution operator, which is this 1 minus i h over h cross delta t, this is the usual time evolution operator in quantum mechanics that you have used to get the Schrodinger equation for the straight vector.

It is based on this essential idea, which describes I am evolution of the straight vector, and now we consider time evolution of a time reversed state. So, you take an arbitrary state alpha have a time reversal, which is denoted by this operator theta, so theta operating on alpha will give you a time reverse state of alpha. And on this you operate by the time evolution operator, so there are two operators operating one after the other.

So, what we expect is that is motion reversal is to mean, what we expected to mean, then theta operating on alpha will give you the time reversal state, and on the time reversed state, if you operate by the time evolution operator. The result should give you the same state as you would get, if you were to operate on alpha by the evolution operator, but through time interval of minus delta t first, and then reverse that state. Now, this is our expectation, if motion reversal is to have certain meaning in quantum mechanics.

So, we demand what must be the properties of theta, which gives us this particular description of the time evolution of a time reversal state or the time reversal of a time evolution state which has been evolved backward in time that is our question. As, to what properties of theta will give us consistent description of these particular equivalents, now alpha being arbitrary, these two operators on the left side and the right hand side must be exactly equal.

This is the time evolution operator, this is the time reversal operator, and here these are written here in the opposite order, but notice this is plus delta t over here, and this is minus delta t. It is not just the two operators, which are written differently one has plus delta t and the other has minus delta t, so let us bring this to the top of the next slide which is this.

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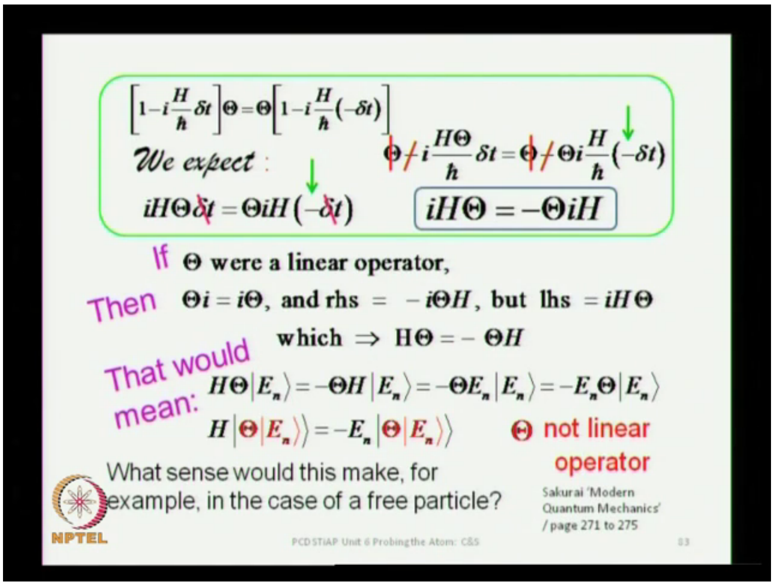

And now you multiply theta with one, so you get theta over here, from the second term you get i h over delta t this is h crossing the denominator in theta. So, everything is written in exactly the same order, and the same thing has been done on the right hand side, do not tamper with the order in which theta and h appear. And do not tamper with the order also in which the square root of minus 1, the imaginary number i is written, it is placed exactly where it is in the first equation, so now cancel these 2 thetas, cancel these 2 minus signs.

So, that gives you i h theta delta t equal to theta i h minus delta t there is a minus sign over here, now get rid of the delta t's, and you get i h theta equal to minus theta i h. And I could have cancelled i on both sides, but I have not done it deliberately, that is what I had cautioned earlier, that do not tamper with the order of i, the reason of course, is that you can pull out the i only if theta is a linear operator.

So, this is the criterion of a linear operator, if theta were a linear operator, then theta i would be the same as i theta, because that i what a linear operator does. And then the right hand side would be minus i theta h, left hand side is plus i h theta, and this would give you h theta is equal to minus theta h. Now, this result would be appropriate, if and only if theta were a linear operator, we could accept it if this could give us consistent results, but does it, so this is what we are led to by assuming that theta is a linear operator.

Then, let us take this result and operate by the operators on the left side and on the right side, on an arbitrary state which is the Eigen state of the Hamiltonian. So, h theta appearing on the Eigen state of the Hamiltonian, let us say nth Eigen state would give you minus theta h operating on the same state. Now E n is Eigen state of h, so it will give you E n, E n is an Eigen value, and what it essentially gives you is E n is a real number, so you pull it out.

And what it essentially gives you theta E n is also an Eigen state of Hamiltonian, belonging to the Eigen value minus E n, we started with en as an Eigen value as an Eigen state of the Hamiltonian with Eigen value E n. And, now, we get the time reversed state also to be the Eigen state of the Hamiltonian, but with a negative energy Eigen value, now would this make any sense consider a free particle alpha is an arbitrary bit.

So, it should hold for any and every bit consider a particular case, where your state is a free particle Eigen state, and how would you have a time reversed state belonging to an Eigen value, which is minus of E n value. What could that mean, it would be nonsense, a free particle has only got positive energy states, there are no negative energy states for a free particle, so this would not make any sense.

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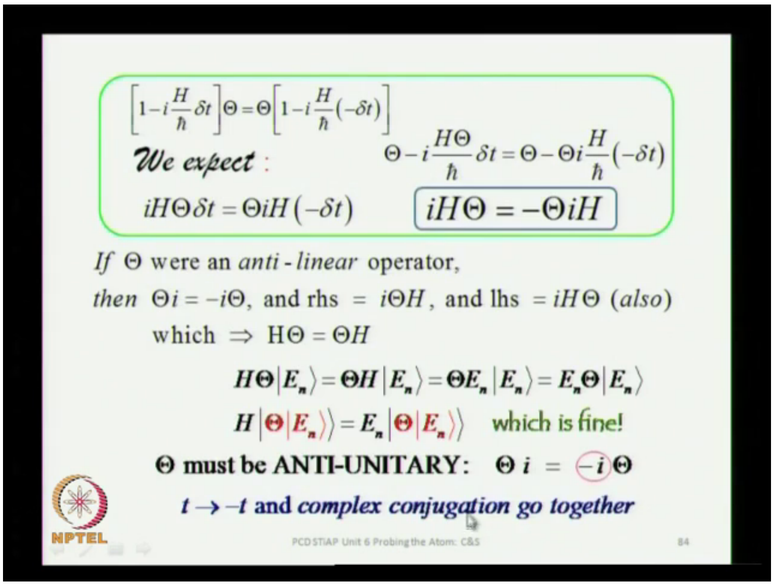

So, the conclusion is that theta cannot be a linear operator, because assuming that theta is a linear operator leads us to an inconsistency, so now just to be careful let us assume that theta is not linear, but it is anti-linear. What it means is when you write i to the left of theta, it would change it is sign. Now, if you did that then the right hand side I would change it is sign, and then you will get i theta h and the left hand side is i h theta h theta equal theta h. And now, you get theta e in time reversed state to be an Eigen state of the Hamiltonian belonging to the same value which is fine, so there is no problem with this.

So, our conclusion is that theta must be an anti-unitary operator, it cannot be it a unitary operator, it cannot be linear operator, it has to be anti-linear operator, and together with the preservation of the norm, it becomes an anti-unitary operator. So, the time reversal operator in quantum mechanics, is an anti-unitary operator, so t would go to minus t, but along with this minus i goes to plus i plus i will go to minus i.

So, there is a complex conjugation which is involved t going to minus t, and a complex conjugation are two immediate and essential factors which are involved in time reversal symmetry in quantum mechanics, they must go together, you cannot just to 1. So, t going to minus t in complex conjugation, they go together in this anti-unitary description.

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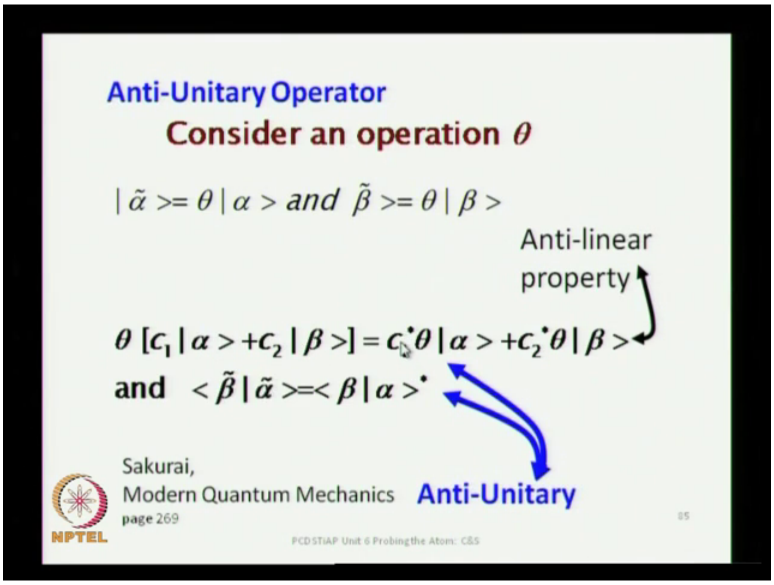

These are the essential properties that an anti-unitary operator, if you have a theta to be an anti-unitary operator, and if it operates on 2 arbitrary states alpha and beta giving you alpha tilde and beta tilde. Then theta operating on a linear combination, c 1 alpha plus c 2 beta will give you c 1 star rather than c 1 in a linear operator, you would just get c 1, but this is anti linear. So, there is an anti-linear property and another property connected with the norm, and that together makes, it an anti-unitary operator in quantum mechanics it has got some interesting properties, which I will not discuss at length, but mention them.

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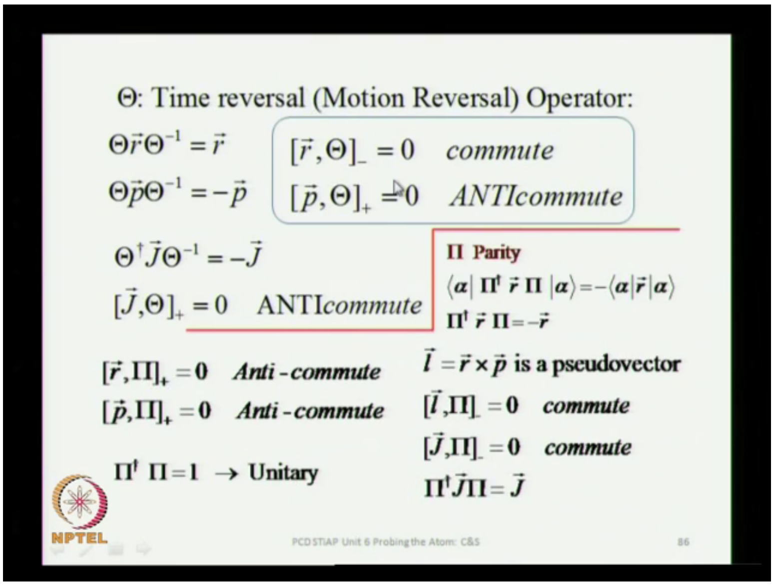

That the time reversal operator would commute with the position operator, but it will anti-commute with the anti-linear momentum. It will anti commute with the angle momentum, but you can contrast this with the parity operator, which is another discreet symmetry in quantum mechanics. And it has got some resemblance, because it has got one of the three discreet symmetry operations of the standard model, so the parity it anti-commutes with both the position and the momentum operator, but it commutes with the angle momentum. Whereas, the time reversal anti commutes with the angle momentum, anti-commutes with the linear momentum, but commutes with the position operator, these are some of the differences of importance.

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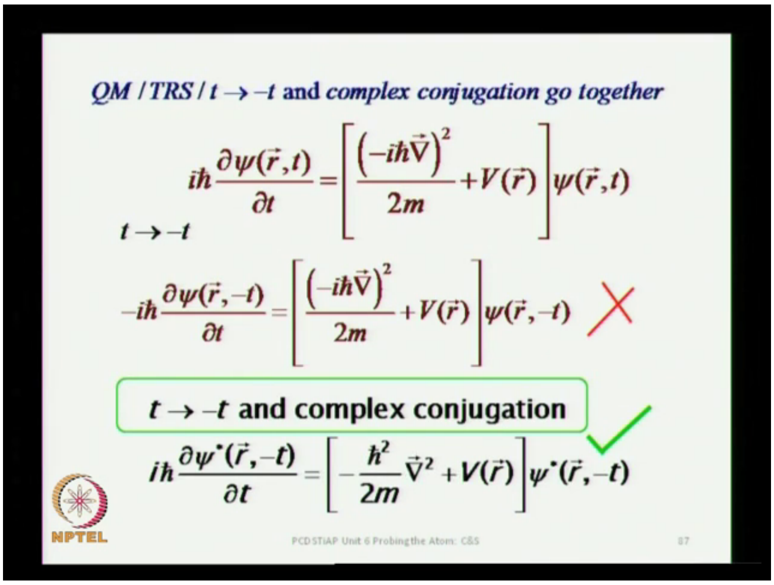

And you can relate to the Schrodinger equation, because if you write the usual Schrodinger equation, this is the time dependent Schrodinger equation. Now, if you just let t go to minus t, then this argument t has gone to minus t, del over del t goes over minus of del over del t, this is what you get from the left hand side. On the right hand side you have got t going to minus t this is what you get, and this equation you get is certainly not like the Schrodinger equation. This is not the Schrodinger equation, but then if from this, if you do a complex conjugation every time, you take a complex conjugation minus i will go to plus i psi will go to psi star.

So, let us do that, so minus i has gone to plus i psi has gone to psi star, and now you get a relationship which is exactly the same as Schrodinger equation, and it is because t going to minus t and complex conjugation has gone together. So, these are the essential characteristic features, which are of importance in the boundary conditions that we are discussing, which connects the solution of the collision problem to the solution in the photoionization problem.

You will see how it is done, and I will illustrate using a single dimensional problem, and then do a three dimensional problem there is a lot that one can learn through this one dimensional problem. There is potential barrier problems, barrier problems that you do in your first course in quantum mechanics. And they are not just exercises in you know just differential equations in solving boundary value problems, there is so much that one can learn from these one dimensional problem.

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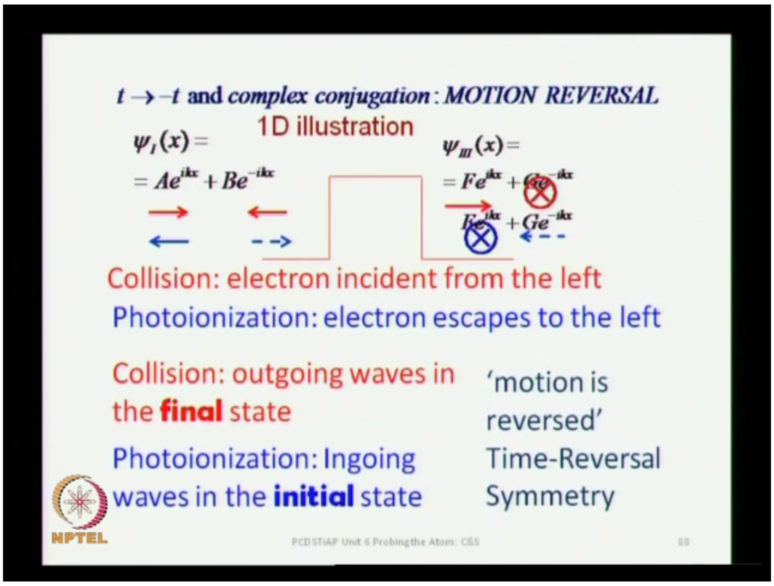

And here is an example, of this particular importance of one dimensional problem, that if you have a one dimensional potential barrier of this kind. And you as always have 3 regions, in region 1 region 2 and a region 3, and then the general solution you write in terms of waves e to the i k x and e to the minus i k x is a linear super position of the travelling waves. You know, which one is going to the left, and which one is going to the right, and you know it because the r time dependence is contained in e to the minus i omega t.

And then depending on how the surface of constant phase propagates, that will decide which will move to the left, and which is moving to the right. So, now, you have got in a collision experiment, now you must relate it to an actual physical experiment, because that is what quantum mechanics is about. That you are trying to describe the collision experiment, this is a one dimensional experiment, you go to the electron, which is incident from the left. So, e to the i k x is the one, which is moving from left to right, and that you know the time dependence is e to the minus i omega t.

So, k x minus omega t is the phase, and constancy of that will require propagation of x from left to right, so you have got electron incident from the left, what can happen to this electron now. It can get reflected, and it can get transmitted, so you can get a reflection here B, and you can get a transmission here, which is the F e to the i k x, this is the wave in the region 3 moving from left to right. And in region 3 you cannot have a wave, which is going from right to left, because there is nothing in the problem, we can send it back again.

So, essentially what this means is that this collision is described in which the electron in the incident from the left, and entrance channel is unique, this is what I have been emphasizing. That the entrance channel is unique in this, then g must be 0 is the boundary condition, which describes the collision, in which the incident electron is incident from the left. Now, in photo ionization, you have an atom you do not have a free electron in the initial state at all, this atom absorbs the electromagnetic radiation, and as a result of the absorption, the electron gets unbound the bound electron like 1 s in hydrogen.

If you give it more than 13.6 volt electron energy, it will become free, it will get ionized into the continuum, now that is photo ionization. And this electron escapes, and it can escape either to the left or to the right in this one dimensional problem, but only in one of the directions, because there is a unique direction for the exit channel. So, let us consider this unique direction to be the electron's escape to the left, so this is the electron escape to the left, this blue line, blue arrow which is escaping to the left.

Now, where was this electron in the initial state, it was not there as a free electron at all, this is not a scattering experiment only in the collision and the scattering experiment, you have the electron in the initial state. So, in this case you can only simulate it by these dash arrows, this is not a real electron, but coming in from both sides to cancel the flux. So, you sort of simulate you pretend that it was there, that is the description, and this description would be appropriate to explain the photoionization process, in which the electron escapes to the left.

Now, what it essentially means is that the coefficient F in this case will be 0, so g equal to 0 is the boundary condition for collision, F equal to 0 is the boundary condition for photoionization. In collision the outgoing wave is in the final state, and in photoionization you have got the ingoing waves in the initial state. So, that is the relationship, and what we are going to see is that these two states are connected to each other by the time reversal symmetry, you expect this. So, if you were to run the film backwards that is the process, you would you can imagine to be seen, so this is the motion reversed state and we will find that these are connected by the time reversal symmetry.

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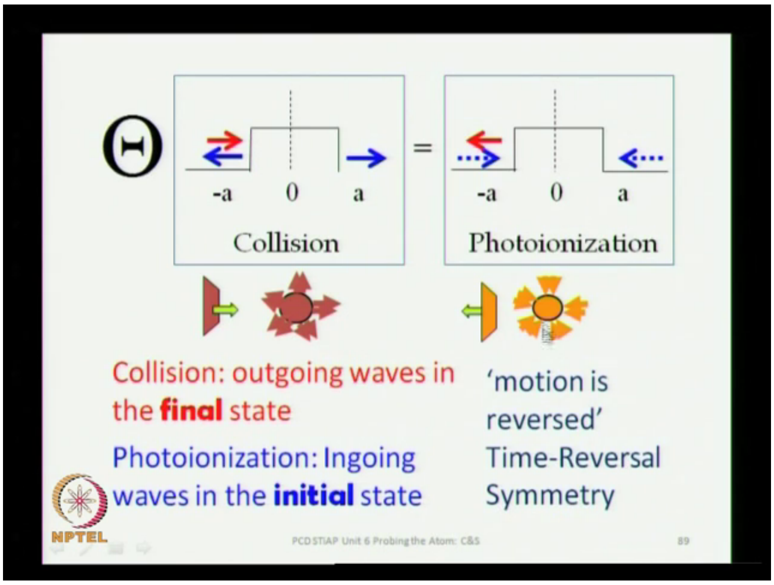

So, if you operate on the collision process by the time reversal operator, you would get photoionization. And sometimes this photoionization is referred to as the half scattering or half collision that is the very common term, which people use essentially, because of this particular connection. So, you have got the outgoing waves in the final state, and this is the three dimensional picture that we expect to emerge, remember these pictures, because they are going to be important.

They will come back in our discussion, when we conclude our discussion of one dimensional problem, we will do the three dimensional problem also. So, if theta operates on this collision experiment, you would expect this photoionization process to be seen as a result of this operation.

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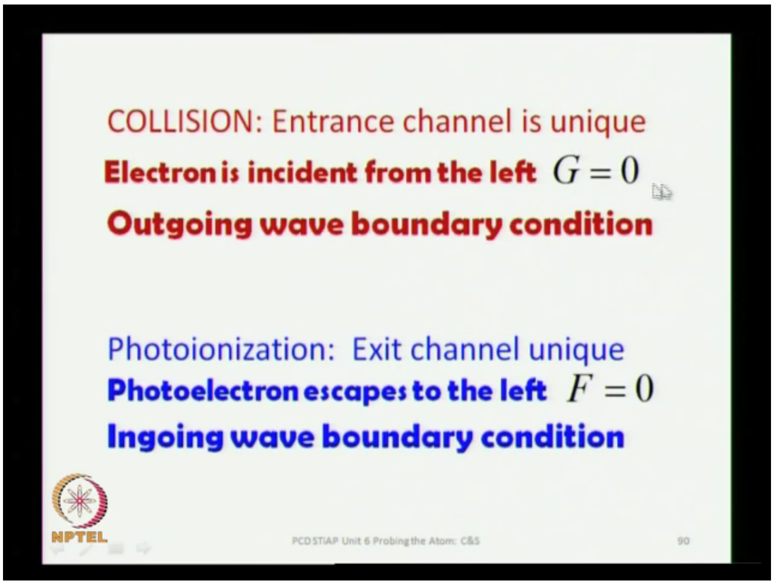

So, these are our boundary conditions g is equal to 0 for collision, and F equal to 0 for photoionization in which the exit channel is unique, in collision it is the entrance channel which is unique.

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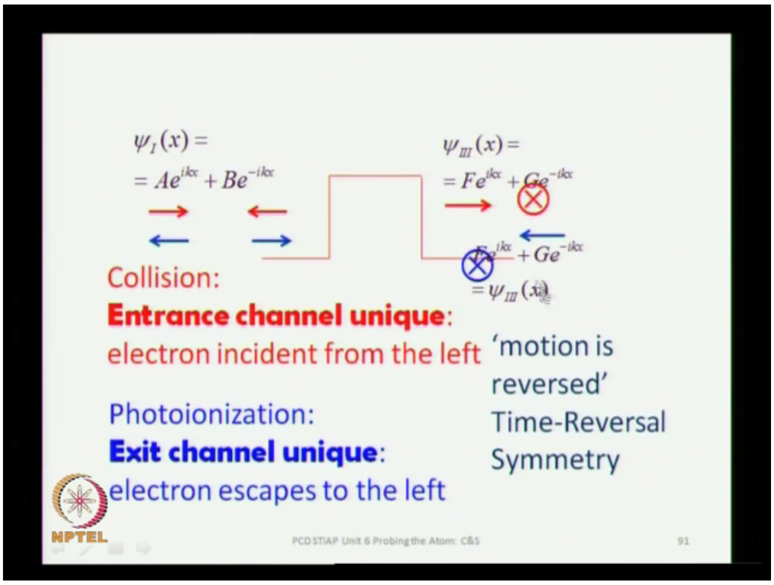

And the conditions are expressed by g equal to 0, and F equal to 0, now I am going to follow the treatment from Fanno and Rau's book, which is a very nice book, which explains these things very nicely.

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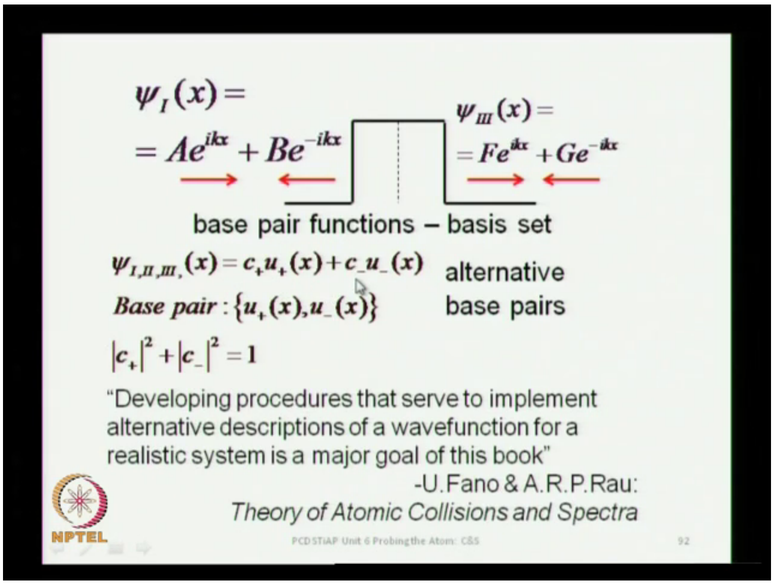

And I have a quote from this book the developing procedures, that serve to implement alternative descriptions of a wave function, for a realistic system is a major goal of this book, because you can express a wave function in any set of bases set. And which bases set is most appropriate in a given condition is a choice, that you are free to make. And you make the best choice, which will bring out the best in physics, like you can solve the problem of the Planetary problem, the Kepler problem.

If you like Cartesian coordinates, you can do it in parabolic coordinates, you can do it in spherical polar or any coordinate system nothing wrong with it, but whichever is the most appropriate which ever gives you the most insight into physics. That is the one you choose, so you would use plain polar coordinates for the two body Kepler problem, and it is a similar kind of situation over here that here. It is not just the simplicity of the equations, what is the most physics that you can extract by making the appropriate choice of the basis.

Mathematically, they are all equivalent, but one gives you a deeper insight into the physics than the other, and that is the choice that you have to make. So, here they propose alternative basis set not just e to the i k x and e to the minus i k x, they can certainly be used. Mathematically, they are complete basis no problem, but you can use any other basis like u plus and u minus with appropriate co efficient c plus and c minus, and you can see what kind of physics you get by making some of the alternative choices.

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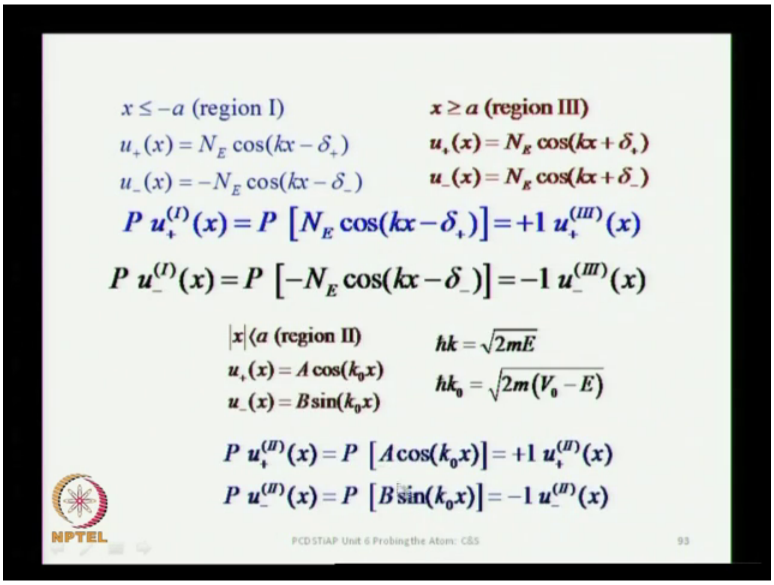

So, here for region 1, they propose u plus and u minus to be given by this cosine functions, but with two different space shift, one has got the space shift delta plus the other has got delta minus. For region 3 you have similar you plus and u minus, and then if you operate on u plus by the parity operator, you find that you get the solution u plus for region 3, whereas if you operate on u minus, you get the negative of the solution for u minus. So, instead of you know travelling waves, you can knew solutions, which connect to the parity operator rather than the free particle hamiltonian.

You can use different kind of basis sets over here, and this particular choice is just for completeness for region 2 also I have given the wave functions over here. They do not appear very much in our discussion, because you are going to see what is happening in the asymptotic regions, which is where the electron gun is where the detectors are, so that is what is most important to the experiment.

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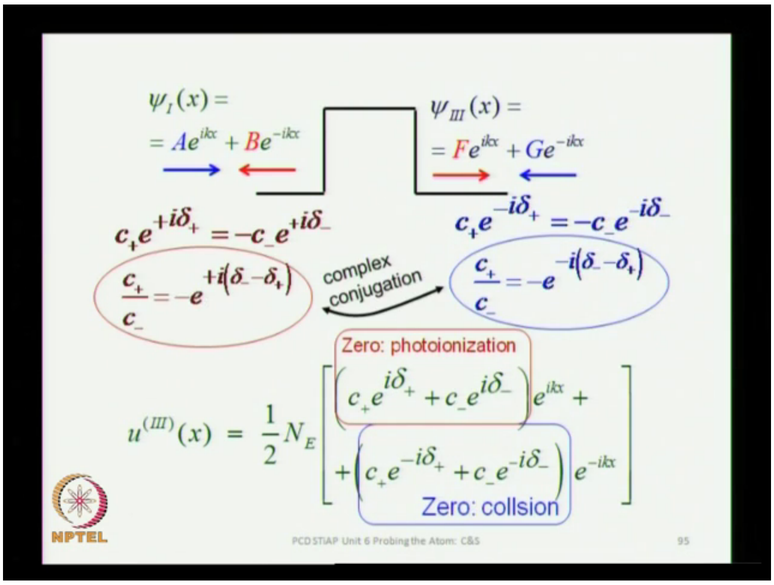

So, now if you write these wave functions, earlier we had used these e to the i k x and B e to the minus i k x corresponding functions over here, the coefficients are now given by these c plus e to the i minus delta plus, because if you just carry out these transformations between the basis set. So, you can write the same wave function in either bases and do the transformation, and this is what you get by doing a little bit of algebra you can do at home. So, you get these coefficients, so this coefficient takes place of A this coefficient takes place of B, if you were to rewrite these functions in terms of travelling waves.

So, you write these functions for the region 1 and also for region 3, similarly and for region 3 these are the this is the linear super position of e to the i k x to the minus i k x, but now to the coefficients instead of A and B are now in terms of the c plus and c minus and the phase shifts. And now, we know that the g is equal to 0 collision experiment, and f is equal to 0 is the photoionization experiment, what essentially it means is that this box will be equal to 0 for collisions.

And this box will be equal to 0 for photoionization, and now let us see how these are related to photoionization. So, let us write this out, so this is the box which goes to 0, in the collision experiment, so c plus e to the minus i delta plus is equal to minus of c minus e to the minus i delta minus. So, this is what you get for the ratio of the coefficients c plus to c minus, this is essentially one phase shift with reference to the other, it is the phase shift difference.

So, you get this coefficient in terms of this difference for g is equal to zer0, for collision what do you get for photo ionization. Photo ionization you get this relationship, let us write it over here, so you get c plus upon c minus equal to minus e to the power plus i delta minus delta plus. What is the connection between two, they are complex conjugations of each other. And this is exactly what we expected, and this connection becomes transparent by making the choice of this basis set, that is the advantage in choosing this basis set.

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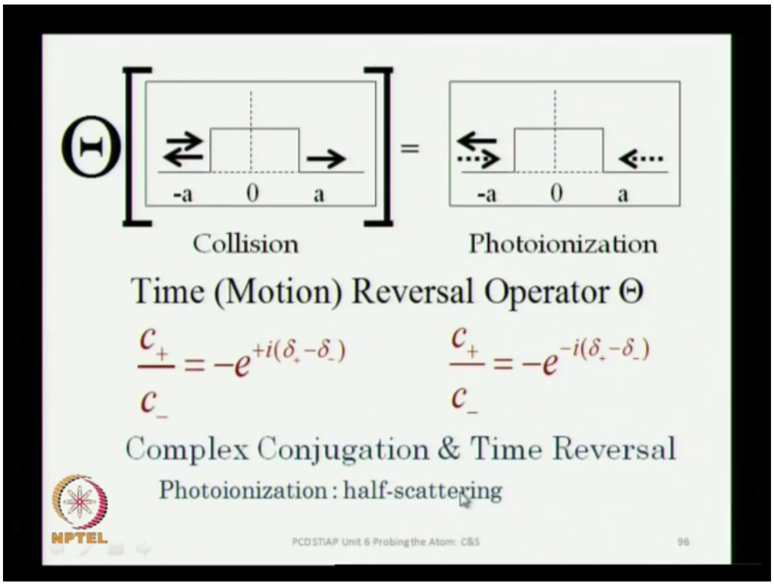

Now, when we are working with this one dimensional problem, I will mention few of the other properties also which can be of importance. So, here I highlight this particular result that the motion reversal that you expect to witness, as you operate on this collision process by the time reversal operator giving you to the photoionization experiment. This relates to the complex conjugation, and time reversal goes together, so this is the essential message from this, which is why I mentioned photoionization is called as half scattering.

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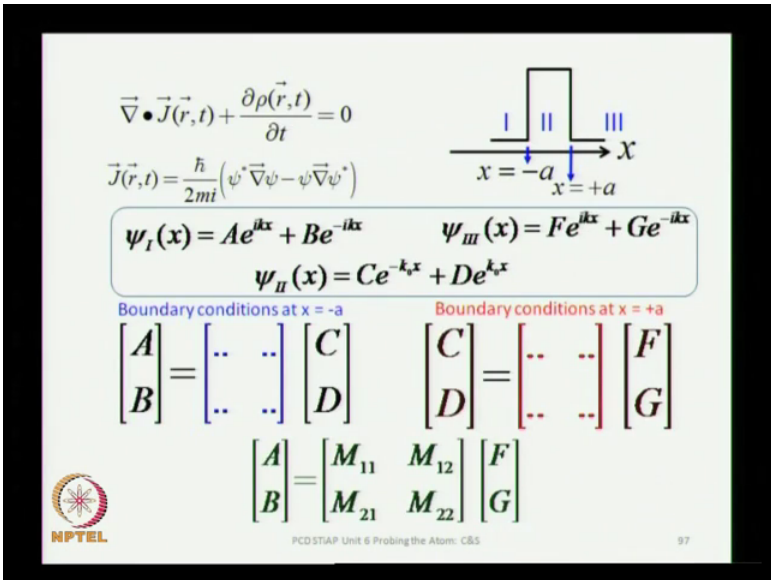

And while, we are at this I will mention a few other learning from this one dimensional problem which are important in this one dimensional theory, you have this region 1, 2 and 3 and you are going to apply the boundary conditions at minus A and plus A. You have the equation of continuity, which is well known to you right the current density vector. And you can get the current density vector for three regions, subjected to equation of continuity, that divergence of j is equal to the negative rate of change of the probability density.

That is which is just the statement of conservation of flux, and then for the stationary states since del rho by del t vanishes the divergence must vanish. And that is what gives you the connections between the coefficients A and B and C and D, and you also get similar connections between C D and F G, so you can write it in a matrix form. So, A is some super linear position of C and D and B is some linear super position of you know, C and D, so these are matrix equations you just have 2 by 2 matrices.

So, I am just writing the structure you can get the actual reflection coefficient, transmission coefficient that you would have done, but then you can eliminate C and D from this, and you will get A and B in terms of F and G. Now, these are of importance, because these are the coefficients in the asymptotic regions, and those are the ones that are of the direct consequence to your source and detectors.

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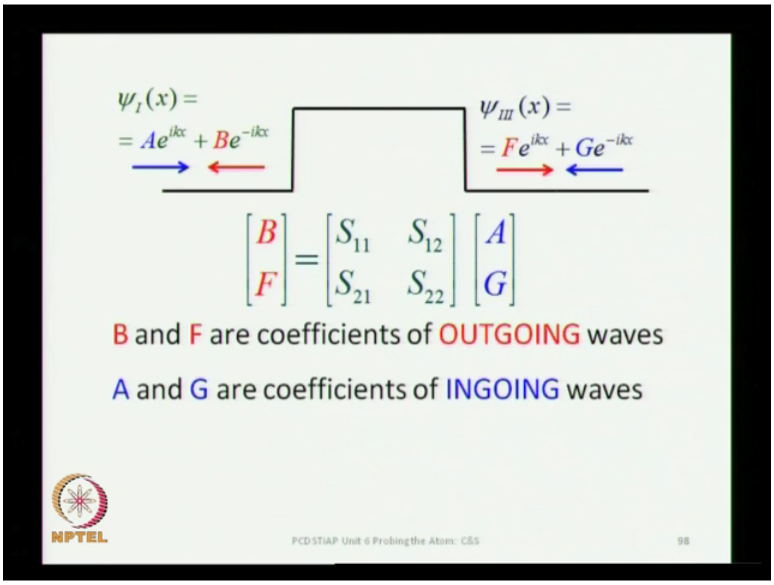

Now, you can do something else my playing with the matrices, you can also write the coefficients B and F in terms of A and G by simply playing with these 2 by 2 matrices. It is just a matter of writing those equations, and instead of you know writing it in terms of the matrix m which I have define it in the previous slide. You write the coefficients B and F, which are the coefficients of the outgoing wave, in terms of the coefficients of the ingoing waves.

Now, this matrix which connects the coefficients of the ingoing waves to the coefficients of the outgoing waves, this is called as the x matrix. And, in fact Heisenberg made did a lot of work developing a formulation of quantum mechanics, in terms of the x matrix formulation. This is the famous x matrix formulation of quantum mechanics by Heisenberg, and this is called as the scattering matrix or the x matrix.

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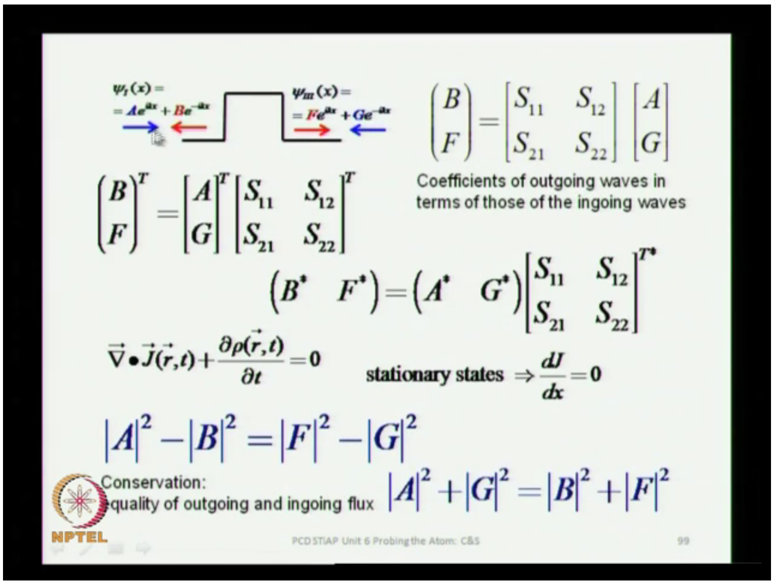

So, you can just set up these two by two matrices, and there is a lot that you can learn from this problem, and you can write this equation for the transpose. You transpose both sides, so t corresponds to the transpose, you can transpose and complex conjugate. So, this is very simple algebra, this is transposition and complex conjugation and subjected to the equation of continuity, for stationary states you will find that the divergence of j is 0, which means that d j d x is 0, in the one dimension. To talk about to set up his equations, you find that the conservation of flux is expressed by this relationship A square plus G square, which is the flux of the ingoing waves is equal to the flux B square plus F square which is the outgoing flux.

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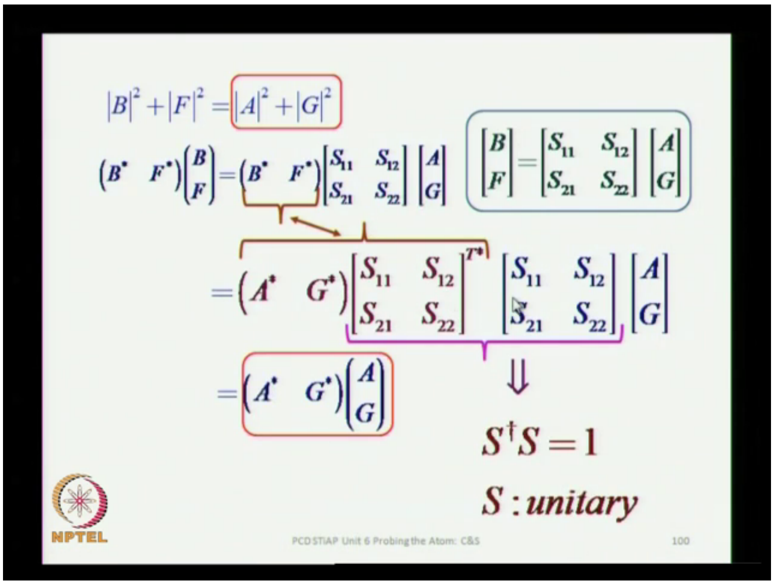

Now, if you see this, now since B F is written in terms of A and G through the scattering matrix, and you construct this matrix multiplication, this is the complex conjugate and transpose of B F this B F is written in terms of this S matrix. So, this is S operator, S matrix operating on this column matrix, A G B star F star is nothing but this and what do you get from here.

Now, this is A square plus G square on the left hand side, and essentially what you get is that the S matrix must be a unitary matrix, so the unitarity of the s matrix is connected to the conservation of the flux over here. And these are some important properties in collision physics, which become handy later on, but our immediate interest in seeing the time reversal symmetry in this process.

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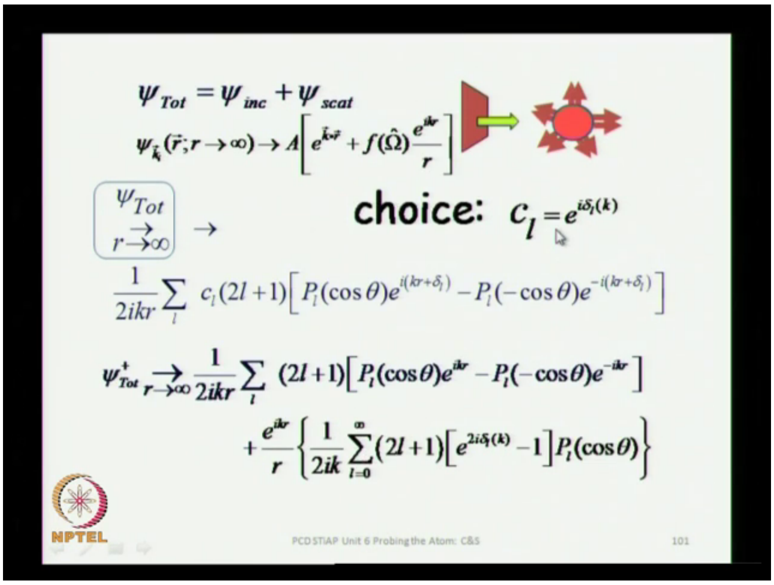

And, we have already recognized, that what we are going to have to do is to, let t go to minus t and complex conjugation together, and we have already seen it how it plays out in the one dimensional problem. But, the problem of interest was the three dimensional problem in which, you can always write the total wave function in terms of these the radial part, we know is the same thing as you get for a free particle, except for the phase shift which is caused by the target potential.

So, you have got a form, which is exactly the same as the plain waves, with the difference that there is a phase shift, which is a scattering phase shift delta l, and these c l's are the arbitrary coefficients. Now, what you would do is choose c l to be e to the i delta e l, now if you choose e to i delta l, c l to the e i delta l, then what do you get. You get the total wave function you put c l equal to the i delta l and you do not forget the scattering scattered part, so it is the sum of the plain incident wave and the scattered wave.

In the scattered wave it is only the outgoing part, which is e to the i k r b by r which has got the phase shift 2 i delta l, and this is the scattering solution for the choice c l equal to i delta l. So, c l equal to e to the power i delta l is the boundary condition, which gives you the correct solution for the collision problem.

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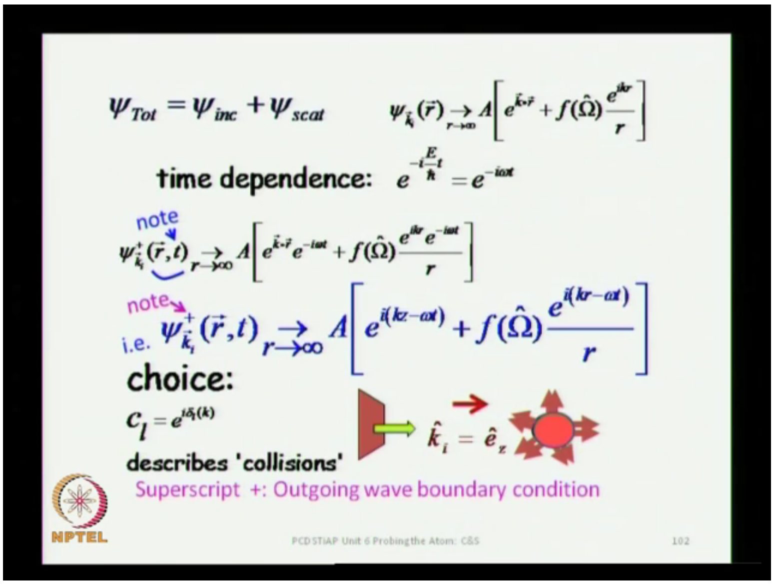

Now, let us see how it connects with the time dependent process that we are really picturizing, because we know that the time dependence is contained in this e to the minus i omega t. So, you multiply everything by e to the minus i omega t, so you have got a time dependent function now, I have written a superscript plus here, to denote that these are outgoing boundary wave conditions corresponding to the collision experiments.

So, here I have got e to the i k z minus omega t, it is coming from here, and here I have got k r minus omega t. So, this is the incident plain wave moving from left to right, this is your collision boundary condition to the outgoing boundary wave condition, and you get the picture that you expected to see. What has given you this picture, just the way you hide g equal to 0 over there, here the choices c equal to e to the i delta l.

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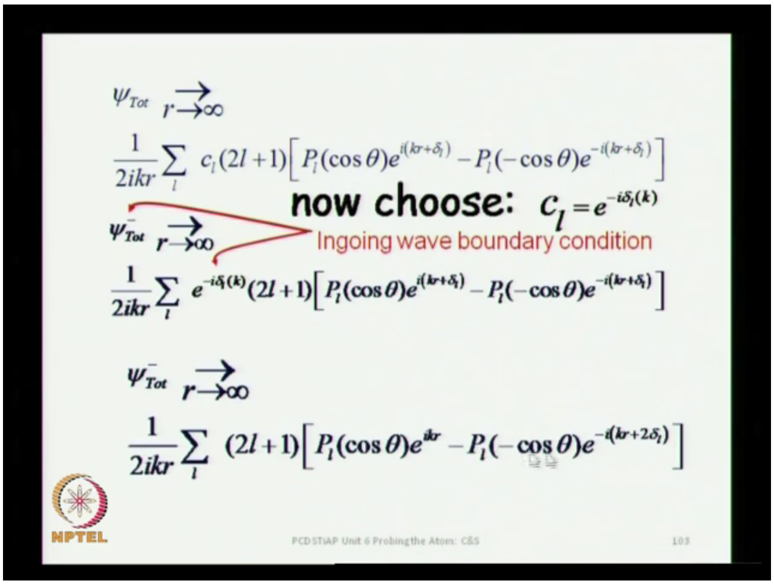

Now, let us rewrite the total wave function, we begin at the beginning, we have an arbitrary solution for the scattering problem with arbitrary coefficient c l, but this time around. Since, we expect the complex conjugation to appear in the boundary condition, we have seen it in the one dimensional problem, we make the choice c l equal to e to the minus i delta l, last time we did e to the plus i delta l.

So, now, what des c equal to e to the minus delta i give you, so this is what is called as the minus ingoing wave boundary condition. This is denoted by superscript minus over here, this is e to the minus i delta l which takes place to the c l, and now you multiply every term by e to the minus i delta l. So, this e to the i minus i delta l will kill this, and it will give you two delta l over here, that is what you get over here, you get a two delta l over here this delta l is killed, by e to the minus delta l this is the total wave function, with ingoing boundary wave condition.

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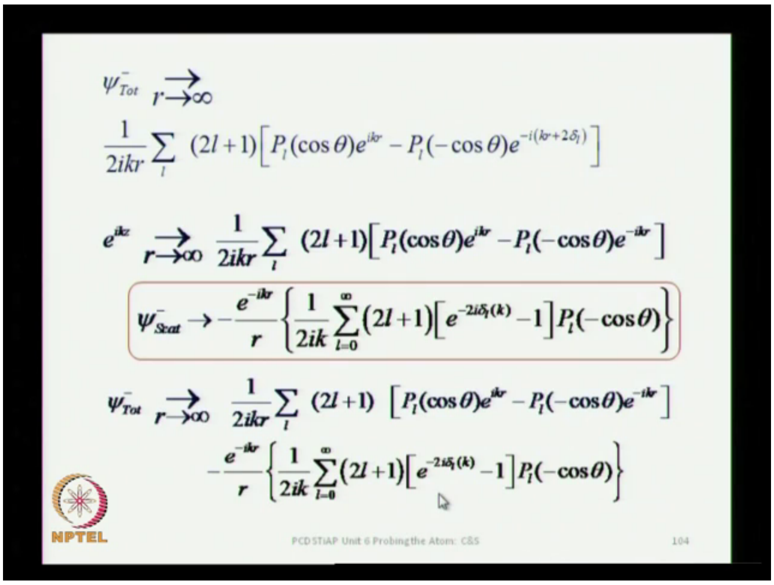

Now, what do you get, you have the incident plain wave, which we have written earlier here in the form already, this is the scattered part, because if you subtract this from the total you will get this part. So, all I have done is to subtract this from this, from the total function I subtract the plain wave, so I get the scattered part, and I write the total wave function as a sum of the incident plain wave, and the scattered part. Now, fair enough this looks like the solution problem, but there are essential differences already, but they will become manifest in our discussion.

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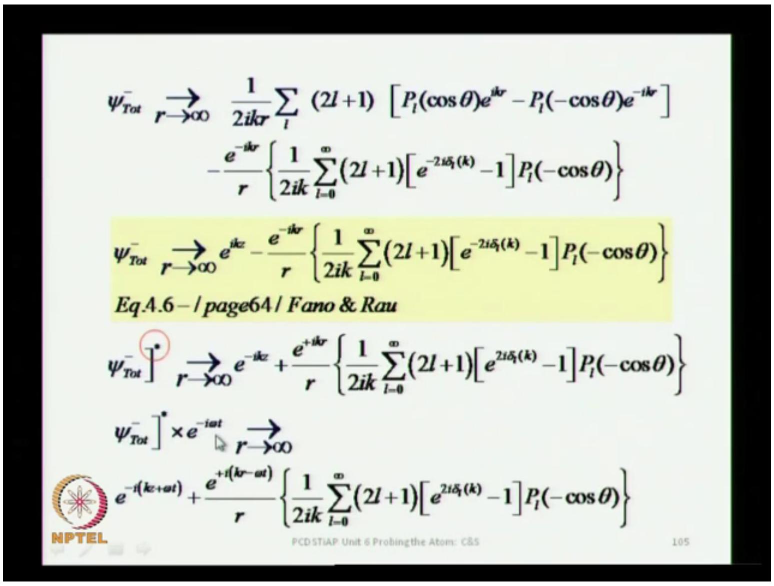

This is the total wave function with the ingoing boundary condition, with the choice c l equal to minus i delta l, this is straight from Fano and Rau's book this is from page 64 of book. And now, we will do a complex conjugation under the t going to minus t, and see what is the picture we get. So, do a complex conjugation, so e to the i k z goes to the e to the minus i k z, e to the minus i k r goes to the plus i k r there is a minus sign here and one over i here.

So, you get a one over I here, but with a plus sign, but that is with a complex conjugation, and this complex conjugation from this minus sign, you get a plus sign, so we have done the complex conjugation. This is the time dependent part which will lead you to the minus i omega t as always, so multiplied by e to the minus i omega t, you get this form bring it to the top next slide as it is.

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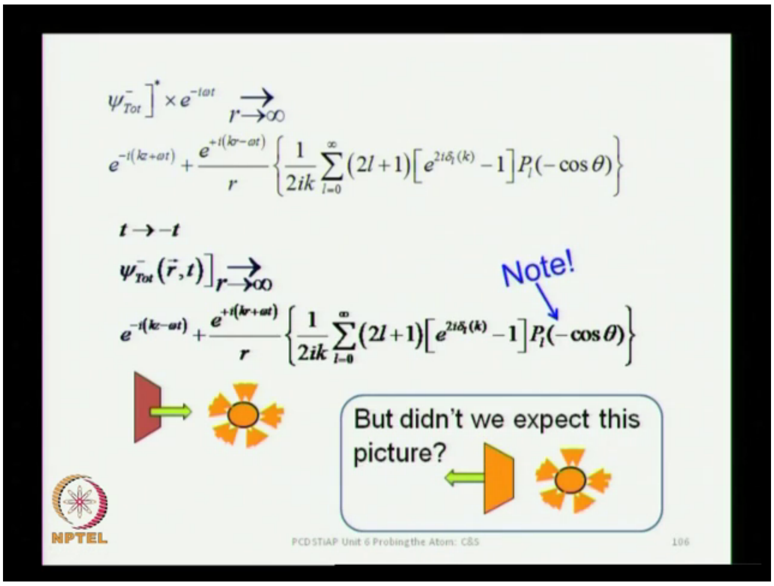

And now, you let t go in to minus t because you have already done complex conjugation, now you let t go to minus t, now what do you get, so you get e to the, so this was plus omega t, this becomes minus omega t this was minus omega t. This becomes plus omega t that is what has happened, everything else remaining the same, and the picture that you get is this is the plain wave, which is moving from left to right. And this is k r plus omega t, now that is what that is a spherically ingoing wave, because of the surface of constant phase will have k r plus omega t will be constant, and therefore d r by d t will be negative.

So, the radius must decrease, which that you are talking about a spherical wave, which is converging to the centre, but this is the picture we were expecting. We were expecting this picture, now there is a difference, and that difference is because there is a factor which some of you might perhaps notice, and some who did not that there is a minus sign here.

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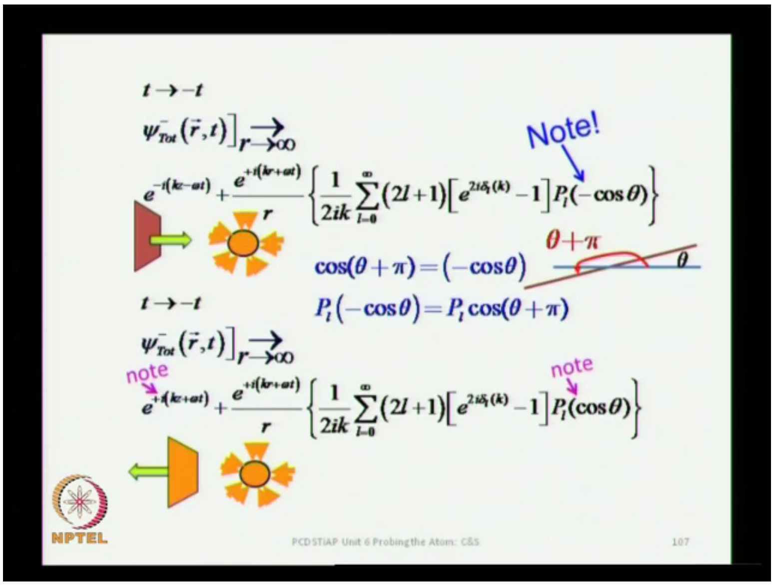

This is the minus sign, which has cropped up in our analysis and it is this minus sign, which I am going to discuss, because you know that if you are going to add pi to theta. Cosine of theta plus pi gives you minus cos theta, so p l of minus cos theta becomes p l of cosine theta plus pi. And this is a big difference, because in collision it is the entrance channel which is unique, so all the angles are measured with respect to that direction.

So, if it is coming like this from left to right, all the angles are measured with respect to this, in photo ionization it is the exit channel which is unique. So, all the angles are to be measured with respect to, there is only one direction with which with respect to which you can measure the angle, which is the direction of the exit channel. And that is going in the minus in the other direction, so z goes to minus z and that is contained over here, that this p l of minus cos theta is p l of cosine theta plus pi.

So, there is a reversal of z axis, and essentially what it means is that the reversal of the z axis will change this z to minus z. And that will give a plus i k z plus omega t over here, and everything remains the same here with this minus cost het becoming cos theta, now, but cos theta is measured with respect to the escape direction. And now, you have the correct picture that is emerging, so the solution to this photoionization problem comes straight from the solution to the collision problem. To the time reversal symmetry all you have to do is let t go to minus t, and have a complex conjugation affected simultaneously.

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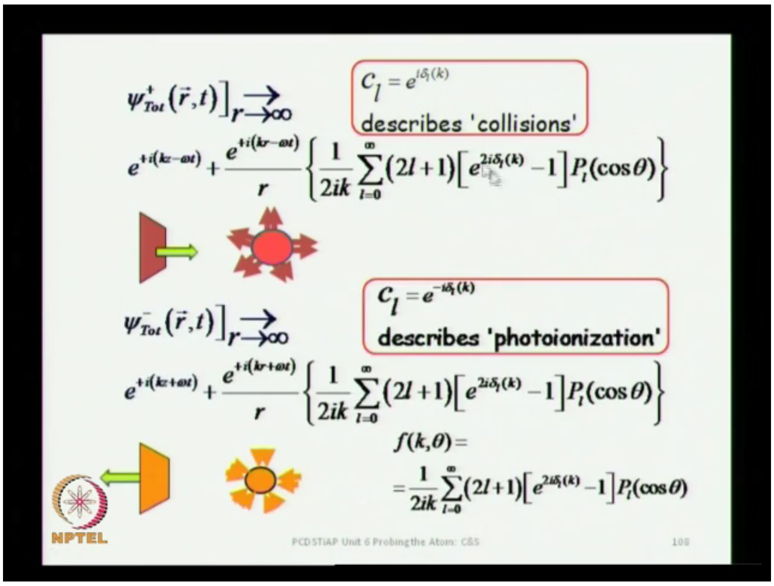

Now, this is absolutely important and this is our main conclusion that c l equal to the i l delta l describes the collision, which is the outgoing way boundary condition. C l equal to e to the minus i delta l describes photoionization, which is the ingoing boundary condition and these two processes are related to each other through the time reversal symmetry.

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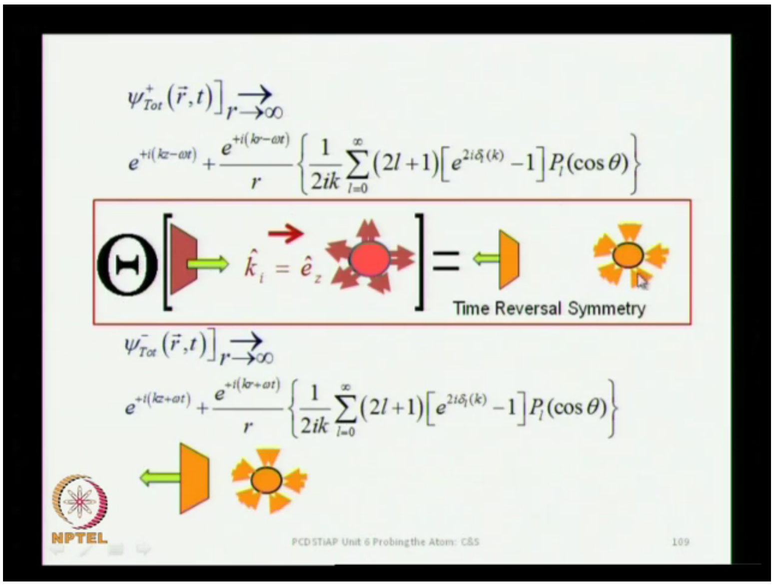

And you have this picture, that the time reversal operator which operates on the collision process gives you the time reversal process, which is photoionization. We have discussed this from the beginning of this unit, that they have got the same final states, but the initial states are different and there is a certain symmetry that connects one to the other. So, the symmetry, which relates them to each other is the time reversal, which involves t going to minus t and complex conjugation going together.

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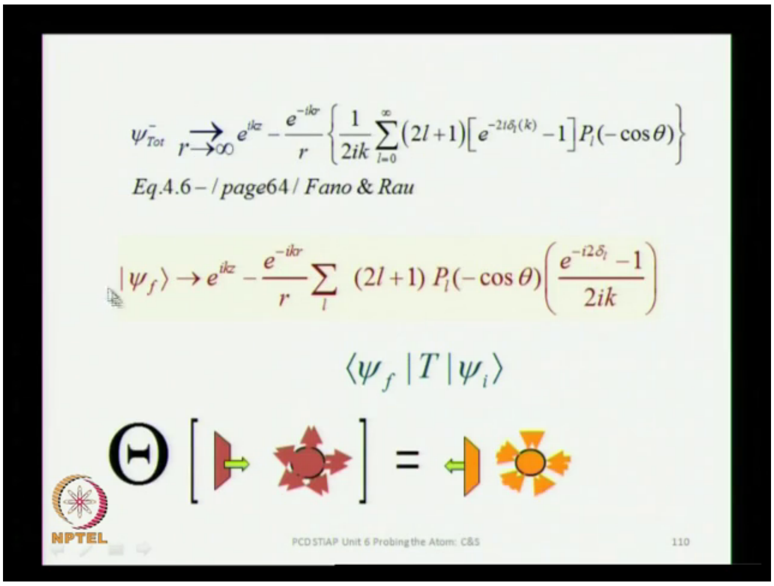

And this is important, because now you get the correct final state solution with the ingoing wave boundary condition, which will be this p l of minus cosine theta, so this is the part that you get. In the scattering solution in the collision it is different, so when you evaluate the matrix element for photoionization, there is a certain transition from the initial state to the final state.

And that matrix element that probability amplitude is represented by this matrix element, which wave function will you put in over here, it must be the wave function with ingoing boundary wave conditions and not the outgoing boundary conditions, you will not get the correct results at all. So, you must make use of these ingoing boundary wave conditions, in describing the photoionization experiment and in the next unit we will describe, how the in what directions the electrons go, as a result of photoionization what is the angular distribution.

So, they do not go necessarily go evenly in all the directions, so when you discuss the angular distribution of the photoelectrons you have to deal with this matrix element for transition from initial to final state. And you must use the correct final state wave function, this is not it is a plain wave solution, but it is an appropriate solution, with correct ingoing wave boundary conditions.

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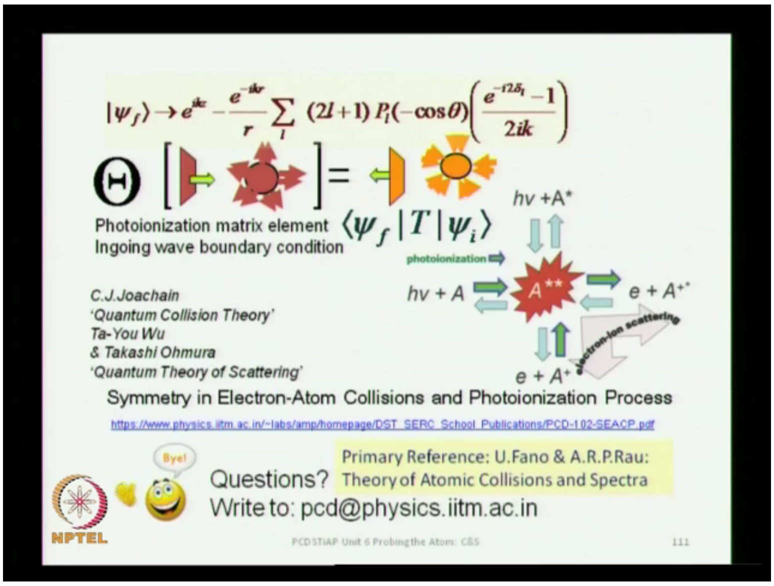

So, this is what must be used and we will be discussing this in our next units, so with this result we conclude our discussion on unit 6, the primary reference for this is Fano and Rau's book, you will also find things in Joachain's book, and You Wu, Ohmura. If there are any questions, I will be happy to take otherwise, in the next class we will go over to unit 7 in which we will describe the photoionization cross section and angular distribution. And we will also use results of time dependent perturbation theory of Fermi's golden rule and so on, so you may have met some of these things in your earlier course of quantum mechanics and we will go through them, because we will require them in the process questions.

Thank you.