Select/Special Topics in Atomic Physics
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Lecture - 32
Atomic Photo Ionization Cross Sections,
Angular Distributions of Photoelectrons – III

Greetings, we will continue with discussion on the Atomic Photo Ionization Process, and particle we will develop the expression for the photo ionization cross section. And it is very complicated to get the exact expression, but we will develop the expression in some approximate limit, which is known as a born approximation.

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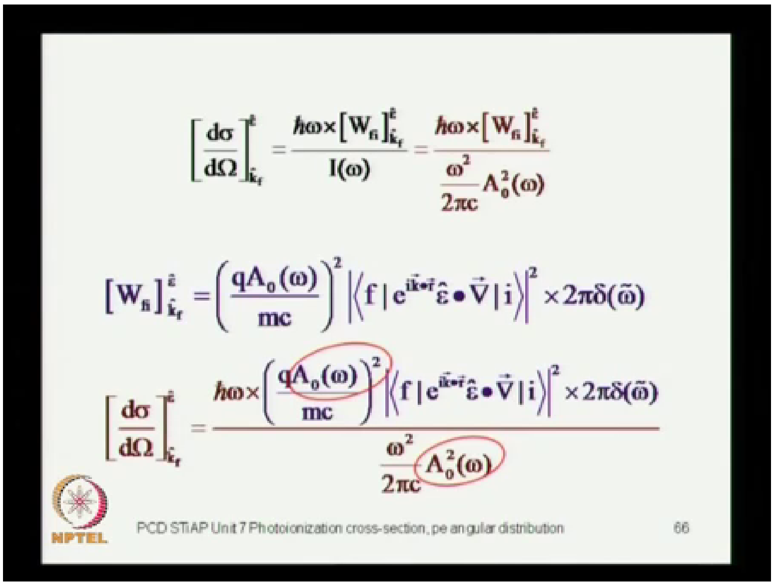

So, we got the expression for the differential cross section in our previous class, which I refer to over here, and remember that this transition rate W has got a dirac delta function over here. So, you must remember that the dirac delta is a quantity, which has got it is own dimension, and you must plug in the dimensions of the dirac delta correctly, so that you will get the correct dimension for the differential cross section.

I have referring to this sometimes, and it is important that you get the correct dimension, so here we have inserted the expression for the transition rate, in the expression for the differential cross section. And notice that there is this square of the amplitude intensity, square of the amplitude of the wave electronic radiation, and you have it in both the numerate as well as the denominator, so these two terms will cancel each other.

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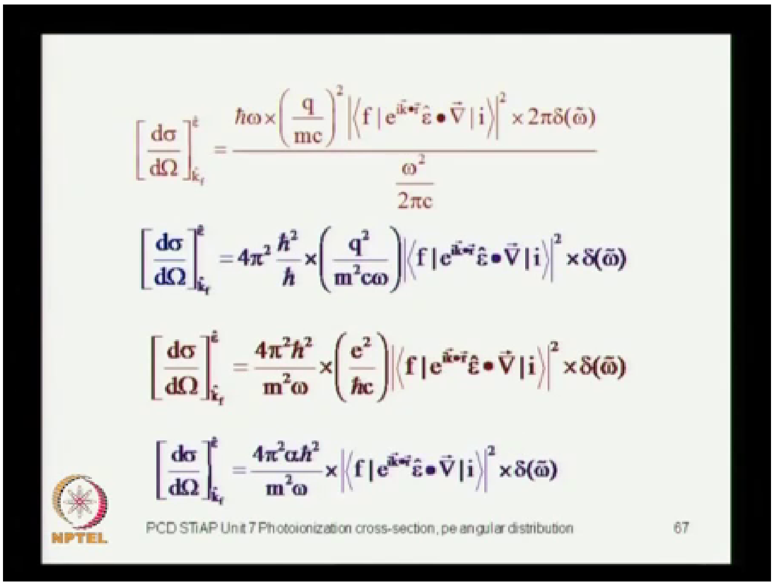

And the rest of the expression is what we have written over here, so the a zero square is gone, and by a slide rearrangement these terms by taking this term omega square, twice pi c to the numerator. You rewrite it in a somewhat convenient form, and extract the fine structure constant e square over h cross c q is the charge, so q square is the same as e square. So, extract fine structure constant from this h cross c, and then you still have an h cross square over here, so this is y h cross a over h cross was written over here.

You have only one power of h cross the first expression, but this allows to extract the fine structure constant, which is the common form in which you will find in literature. That the differential cross section per unit solid angle, for a given incident directions which is pull lies along the unit vector epsilon for photo electronic junction, in a unique exact channel which is along the wave vector k f is given by this expression, so that is what we get for the differential cross section.

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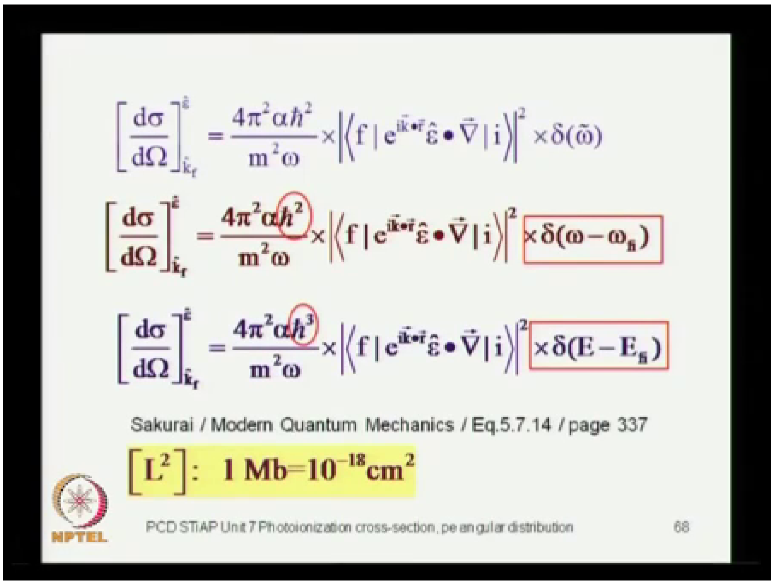

Now, here this omega tilled up is the difference between these two frequencies, now you can write this dirac delta, as in terms of the energy difference as well, because this frequency being equal to the resonant frequency. This condition is precisely the same as the energy of the electromagnetic radiation been equal to the energy difference between the initial state, and the final state. With the dimension of the dirac delta for delta omega and delta e are; obviously, different, which is why you have an h cross q over here as the post average cross square in the previous step.

And this is really important, because in different books whether you look at circular book or shifts book or land left shifts and so on, sometimes you find the differential cross section to be written. And you find a term in h cross square, sometime you find a term in h cross cube and; obviously, you have to keep track of the exact power. And in some literature the dirac delta is not explicitly even written, because it is understood that the transition will take place at a precise resonant energy corresponding to the energy difference.

So, you have to see what the author has in mind, and then make sure that you get the correct expression for the dimension, this dimension when you take all the dimension correctly. It will affect not only the dimension, but of course, the number because you have got an extra h cross over here. So, it your answer will neither be correct numerically nor will have the correct dimensions for the physical quantity, that you valuating it could be observed, so make sure that you always keep track of the dimensions.

And here you will have the dimensions of l square, so it is a cross section, it is not dimensions of area and it is usually reported in units of 10 to the minus 18 centimeter square, which is called as mega bar. So, that is the unit in which the cross section is usually report, and one mega bar is 10 to the minus 18 centimeter square.

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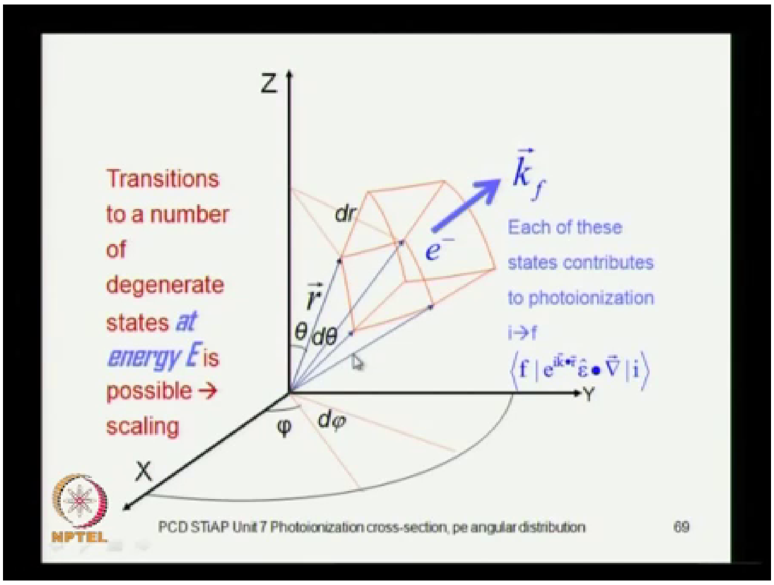

So, now, this is the process that we have consider, we have got the photo electrons which is ejected along this wave vector k f, but then remember that in this direction, there may be other energy states, which are degenerate with the energy at which the transition is taking place. And therefore, this is not unique transition, there will be scaling because there will be if there are additional states, which are at the same energy, where photo ejection in the same direction can take place.

Then you will have to argument the expression for the differential cross section by the number of states, which are available, so we have to figure out a mechanism to estimate this number of addition state, so that we get the correct scaling factor. So, all states which contribute to photo ionization they will all contribute to this matrix element, if they are at an energy which is degenerate with this at this particular angle of rejection.

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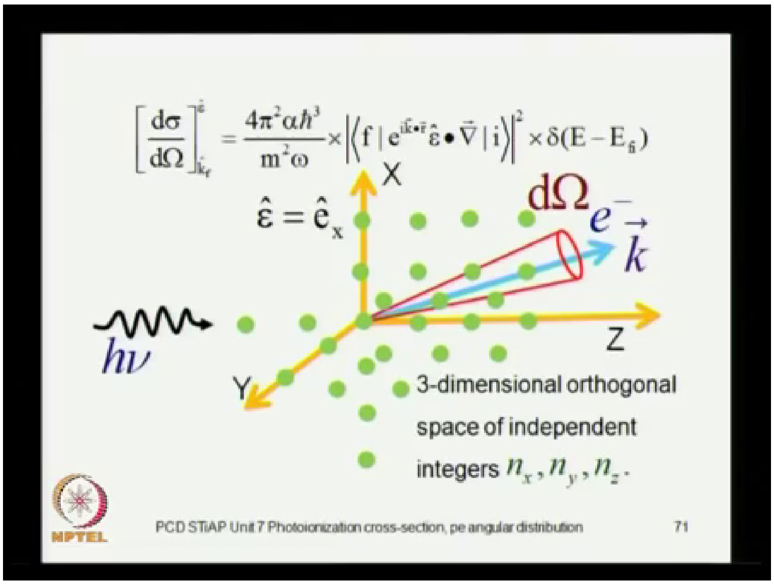

Then what we have to do is to find out this number, so how do we find out this numbers, so what we do is we have to construct a grid of points, so that each of these axis like x axis y axis and z axis instead of looking at axis them is length axis. We consider them to be 3 orthogonal axis the number space, so you have got n axis x along 1 axis, and y along the orthogonal axis, and z along the third axis. And then you construct a grid of points, so what the originate 0, and then you construct a number of points, so you have got 3 orthogonal number axis.

And then you go ahead and put additional points at not just 0, 1 2 3 on the n x axis, but then when n x is equal to 1, and y axis is equal to 1, and z is equal to 1 and so on. So, you get an additional number of points in all coming from all the 3 axis, and then all of these points, which belong to that unit volume, which I showed in the previous figure, all of these point which correspond to that unit volume in the previous figure. So, those are the number of point, which will contributes to the photo ionization process, and the differential cross section will have to be augmented or scaled by this factor.

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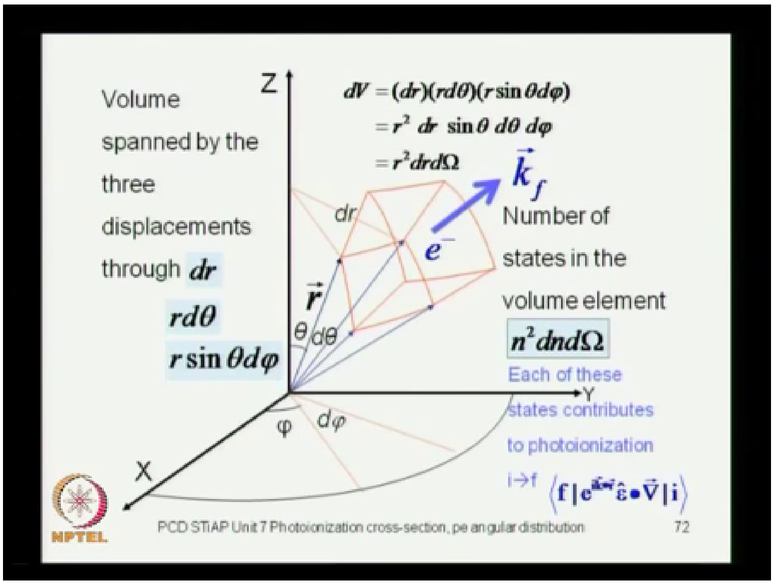

So, how do you calculate that, so you know that the volume element along this axis is given by this r square d r solid angle sin theta d theta define, this spherical polar co ordinate system. And here instead of r you have n, so where n it is a discrete number it is not a continues variable like distance, but for our practical purposes, because all of these points are very densely part, you can treated as a penti, as a semi or a quacy discrete, you know kind of parameter.

So, the number of point that you are really talking about the number of states, which belongs to this volume element will be not r square d r d omega, but n square d n d omega. So, that is the number of states, which are available for this transition, and each of these will contribute to photo ionization corresponding to the same matrix element, because they are all having the same physical energy. So, they are all degenerate processes, at they will actually argument the differential cross section.

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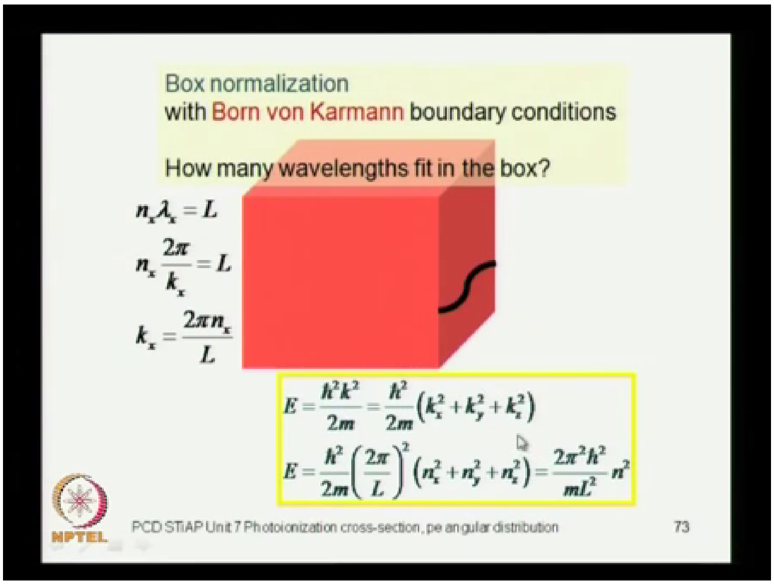

So, to get this number n square d and d omega, the make use of box normalization, and this is tentative one can use other ways one can do other normalization, we have use dirac delta normalization, but you can also do box normalization. Our n result will be independent of the normalization, so you will find that the normalization, really goes off in the final analysis, but. So, this is just a tentative step. And we just use the usual Born Von Karman boundary conditions, and ask how many wave links fit in to the box, because you have these continuum states which are not square integral.

So, we will do a box normalization for these states, and because of this boundary condition, you have the wave number k which goes as 2 pi n over l for each dimension x y and z. So, your energy at which this physical processes taking place, which goes as h cross square over 2 m and k square is k x square plus k y square plus k z square, but k x k y and k z are. Now, given in term of n x n y n and z and the size of the box, so this is what allows you to write the energy as in square times the rest of the constant factor, L is the length of the box, but it will disappear from our final result.

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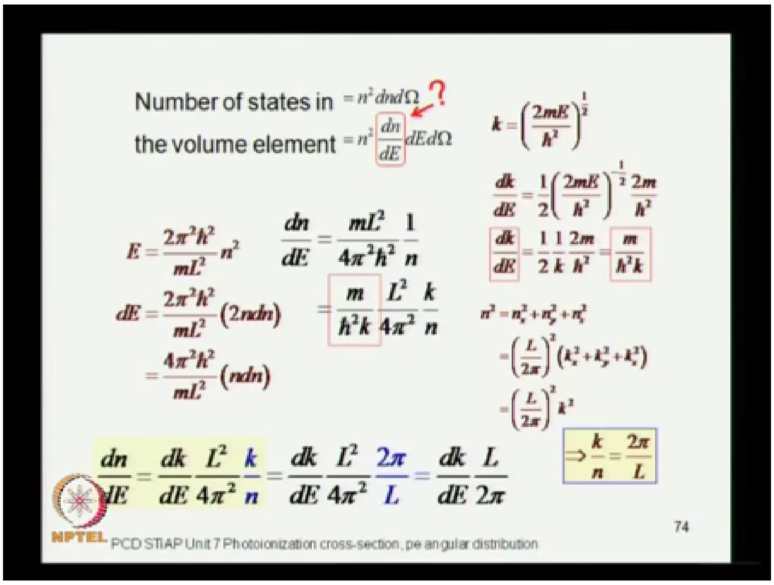

So, this is the number of states, in this volume element we must use, now we need to find what is d n by d e, d n as i mention this is been treated as a quasi descript parameter. So, to get e to get d n by d e you recognize that e goes as n square, so that lets you determine d e in terms of you know, this is the differential in energy, so this will be twice and d n coming from this n square. And now you have d n by d e which you get from this expression by turning this around, and d n by d e goes as varies constants, and then I have extracted the 1 over n.

I have written in terms of k over n, but then k is cancel by this 1 over k over here, because this factor m over h cross k is given by d k over d e, because for a free electron this is the relation between k and energy. So, d k over d e for a free electron turns out to be m over h cross k, so you can write this not just as d n over d e, but you get d n over d e in term of d k over d e n, you will see that this gives as a certain convenience.

So, d n over d e is what you get from here, so d n over d e comes out in terms of d k over d e times the other parameter, but there is the k over n that sticks out. And you need this k over n, and you may get the k over n already because you have this expression between n square and k square, so k over n is nothing but twice pi over l. So, you use this expression for k over n and this is twice pi over l, and now you have got and l square over 4 pi square at the 2 pi over l, so that gives you l over 2 pi, so this is the expression for d n over d e that should go over here.

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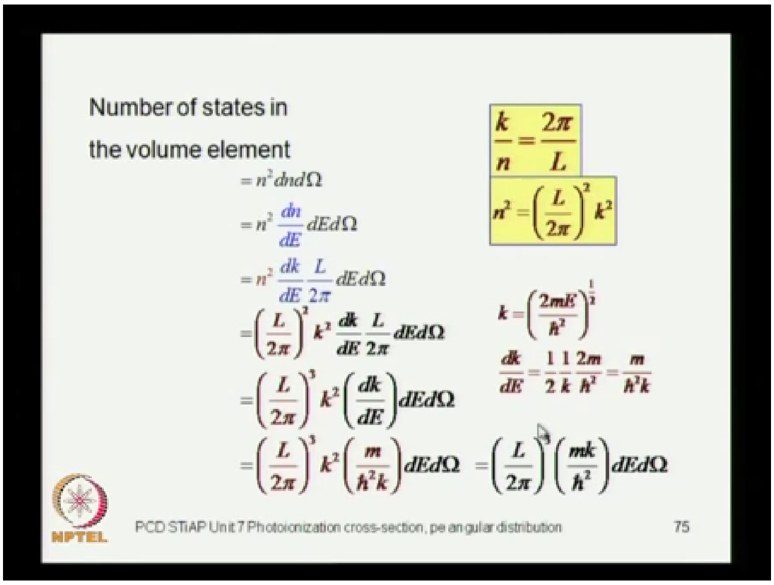

So, we have put that n over here, and given the fact that n square goes as k square, this n square is now written as l square k square over 2 pi, so that is the only substitution over here, very straight forward substitution. And now you can combine this l over 2 pi over here with the square of l over 2 pi, so that gives a cube of l over 2 and then you have k square d k over d e d e d omega, and given again the fact that d k over d e as I showed in the previous slide is nothing but m over h cross k.

So, you can write this over here, and then you can always simplify this, so that you have the cube of l over 2 pi, and then you have one of the powers of k and so this in the denominator. So, a what 1 power of k in the numerator, you get m k over h cross square d e over d omega, this is matter of some detail, but it is important to do it.

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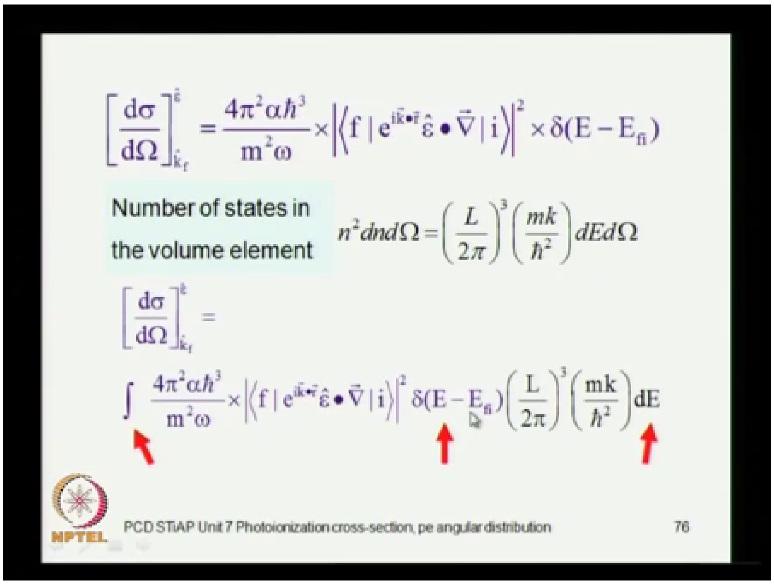

So, once you put in this n square d n d omega, which we have found we need to add up the contribution due to all of these states, which are degenerate with respect to the physical process that we have in mind. So, you have to add up and addition is integration, so that is what we have done over here, you got this dirac delta this integration is over the energy.

And you can carry out this dirac delta, after scaling it by this additional factor, and now you do a dirac delta integration over this, so you will get you know how dirac delta function is done. So, you will get the integral only for the particular value of e, corresponding to e f i, so that is the only term which will contribute and that is what you get over here.

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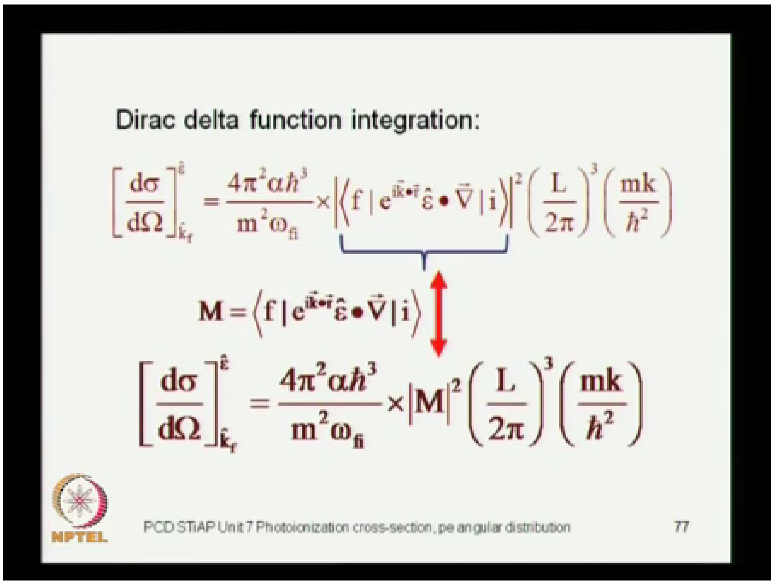

So, e equal to e f i will correspond to omega equal to omega f i, so I am now putting subscript on this omega, which is coming from e equal to e f i, and then you have some of these additional terms. So, this is the expression for the differential cross section for unit solid angle, and it already takes into account the augmentation due to the additional number of states, which are degenerate with respect to energy, at which photo ionization is than the consideration.

So, now, we are going to have to take some specific interest in this matrix element, this is the matrix element of this operator between the states i and f, which have written as m you have the square of the modules of m, which I have written here. And we will discuss the implications of this matrix element, which is the transition matrix element for the transition for the initial state to the final state.

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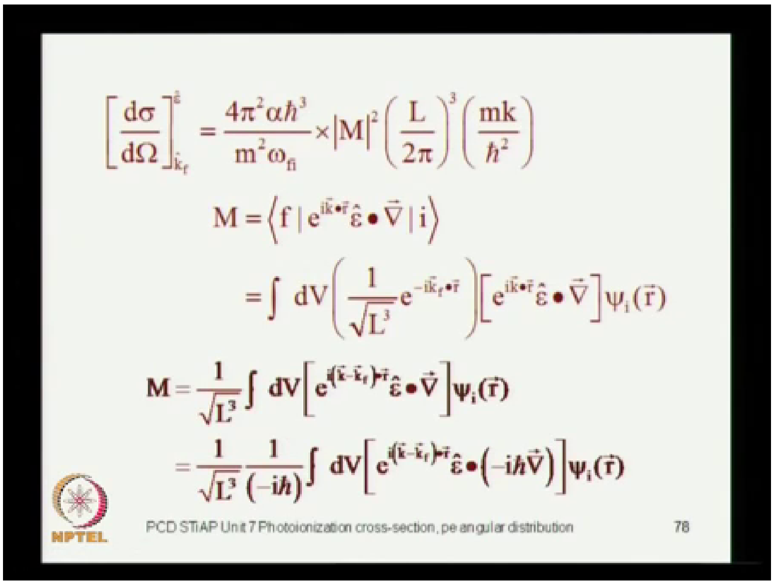

Now, notice that this matrix elements is essential a spacing integral, this is the dirac notation it is essential an integration over space, so let us write this explicitly as a space integral. And now, you have the continuum state which is again box normalized, so got the one over root l cube coming for this, so you have got the continuum state f as e to the minus i k f dot r.

And then you have got e to the i k dot r, which is over here you have epsilon dot l, and then you have the initial state wave function, I do not know if some of your beginning to recognize the form of this function, because it is developing into an integral, which is a very famous expression in mathematical physics. So, this is the matrix element, and you now extract this 1 over root L cube outside, you got the rest of the integral, and in this integral you have the momentum operator gradient. So, to write this del operator is a gradient operator multiplied by minus i h cross, and also divided by minus i h cross, so that in the matrix element, you recognize that you really have to get the matrix element of the momentum operator.

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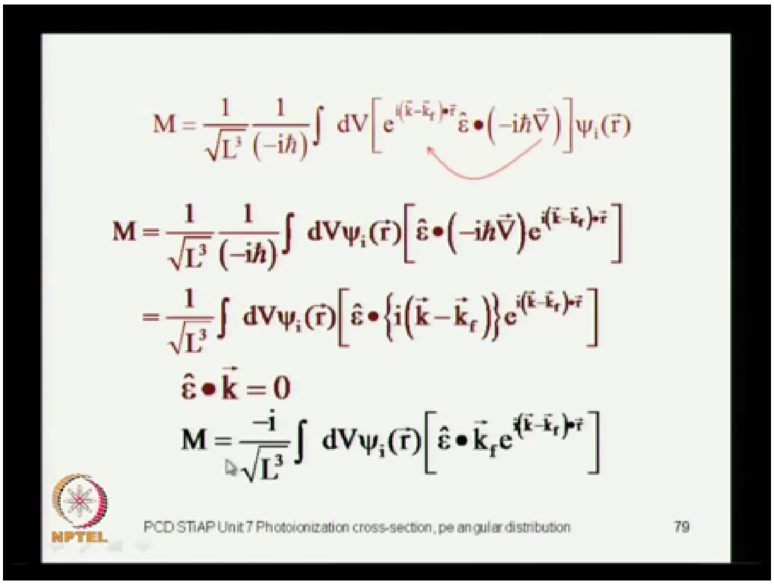

And, now you that you have got this gradient operator in the integrant, this is the momentum operator, which is a exponential operator you, so you can have it operate on the right are also on the left effectively. ((Refer Time: 17:57)) operate on the left, because we know what is the gradient of this k minus k f dot r, this is the very simple derivative of an exponential function. So, you have it operator on the left rather than on the right, and then when you do that when you operate it on the left you get epsilon dot i k minus k f, this is the k minus k f.

So, this is the term which is coming in, when you operate it on the left, and you have the to multiply by this pi i which is written over here. So, this is the matrix element, and now epsilon dot k minus epsilon dot k f is what you need, out of which epsilon dot k is 0, k is the direction of propagation of the incident electromagnetic radiation. Epsilon is the polarization which is orthogonal to that, so epsilon dot k is 0, and now instead of this k minus k f, you only have epsilon dot k f is a minus sin, which I have written over here, so this is your expression for the matrix element.

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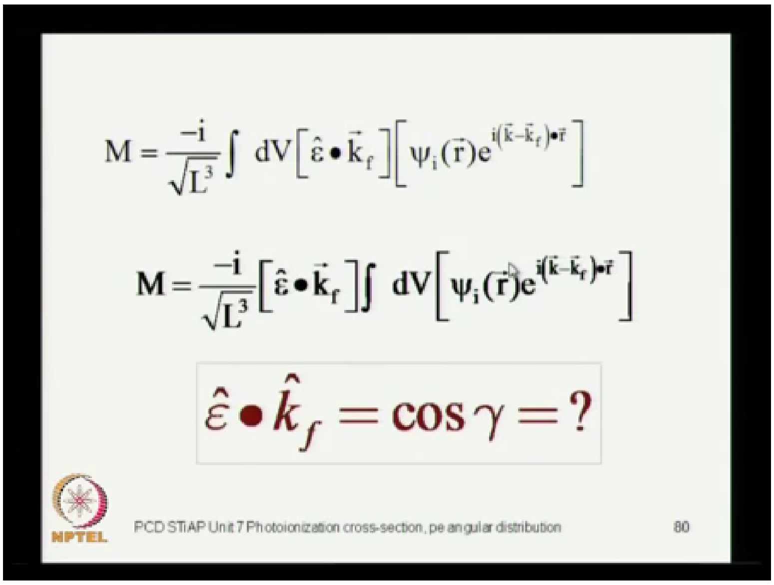

Now, this is epsilon dot k f, now photo ionization takes place on a unique direction, so epsilon dot k f with reference to this particular unique exit channel is a certain constant cosine terms, which you can pull out of the integration sin. And the rest of the integral you will see that, you need the cosine of this angle, other than the magnitude of k f, of course,, but then you will need the cosine of this angle, and then you will have to evaluate this integral.

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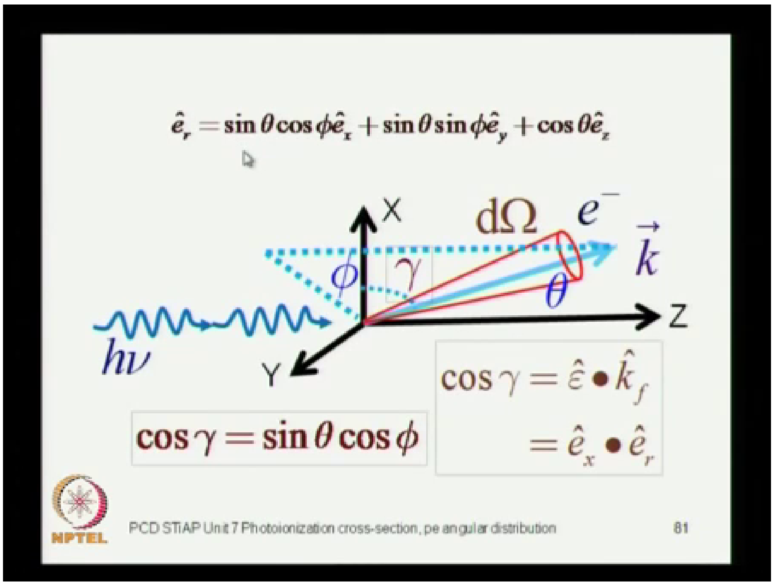

So, what is the cosine of this angle, this is the angle between the polarization vector, which is along the x axis and k f is the direction of reduction, so you can get it easily by taking this unit vector is along e x. This is along the spherical polar unit vector e r, so you can write e r in terms of e x e y e z, and then take the scalar product of e r with e x, so you see that this cosine term is nothing but sin theta cosine phi.

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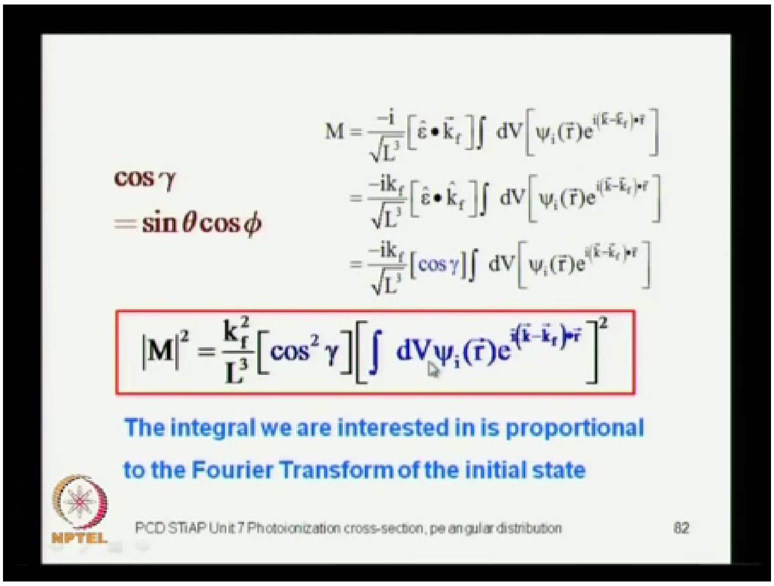

So, that is what you get for the cosine term, and now you can use this cosine term, in the expression for the matrix element, this is what we have determine the cosine term. This is sin theta cosine phi, and this is cos square omega, when you take the modules square, and then you will have to take the square of this integral is well. So, this is a put the whole integral in this rectangular square brackets, and then I take the square of it and when I take the modules square. So, you get l cube over here, and you can see how the box normalization l cube will cancel, what we had originally soughed out it.

So, the integral that you looking at, this is essentially the Fourier transform of the initial state this is the what I did not it, that it is developing into an integral, which is very commonly use in mathematical physics. This is nothing but the Fourier transform of the initial state, and for any initial state all the hydrogen atom, you know 1 s to 2 s and. So, on, all these functions are well known. You can get the Fourier transform very readily, so that is the result that you can plug in straight away.

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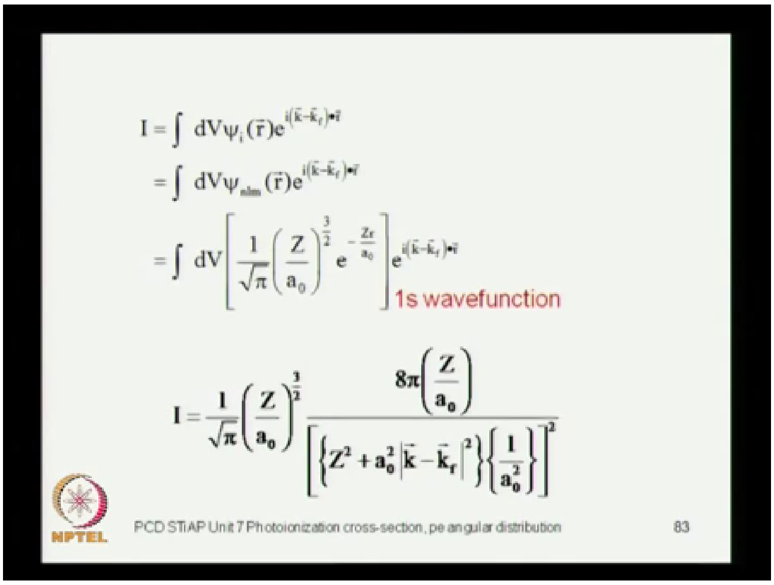

So, what you can do is just for the sake of consideration, the initial state could be any initial state with quantum number is n l and m, just to illustrate this physics, which is contained in this expression. I will use photo ionization of the hydrogen atom in the one state, so this psi n l m is nothing but the one state of the hydrogen atom, and what you need is the Fourier transform of the hydrogen atom one a state.

So, this integral which is the Fourier transform of the one is state of the hydrogen atom, this tells out to be this which is the matter of mathematical details, just matter of getting the Fourier transform of the one is wave function. So, this is what the Fourier transformation gives, you and we will use this result in getting an expression for the matrix element.

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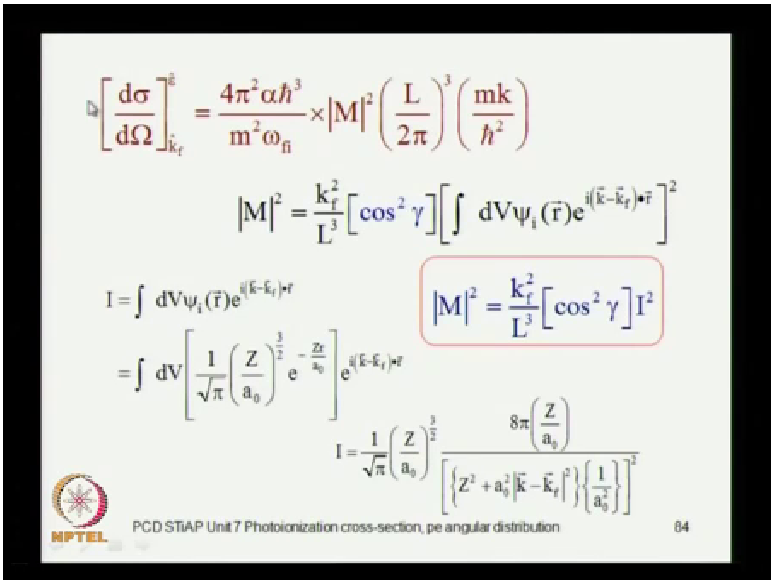

So, the matrix element square is what you need you have this integral, which need to be determined this is the Fourier transform, at this integral which is the Fourier transform is having this form. So, you will plug in this integral in the expression for the square of the modules square, this will go over here, which will go into the expression of the differential cross section, so it is just a matter of substituting the corresponding term that is what we doing.

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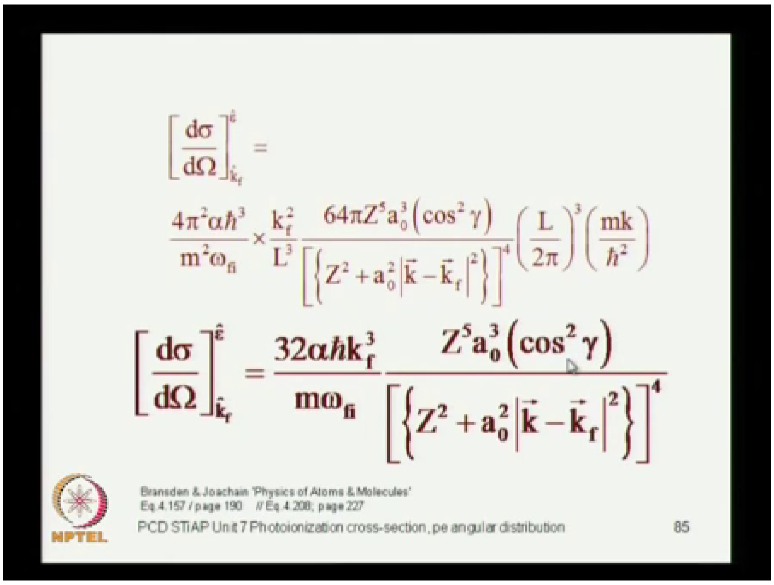

So, let us do that once you put in the Fourier transform, the differential cross section, and I am carrying this information about the direction of spoliation, and the direction of photo ionization by writing this superscript and subscript over here. So, this is a complete expression that you get notice that, this l cube will cancel l cube, so the size of the box really does not matter, and the box normalization that we done there is nothing arbitrary about it, because it really does not matter.

So, now, you can cancel all the terms, and then you have various term that you can combine, so l cube cancels l cube and you had a 64 over here, but there is a 1 over 22 the power of 3. So, there is a 1 over 8 here. So, this 8 64 by 8 into 4 is what gives you this 32, so you get this 32 alpha h cross, then there is the k f cube coming in, there is k over here, this is taking place at the resonant frequency. So, you got a k f cube over here, and you got the cos square distribution as we have noted already.

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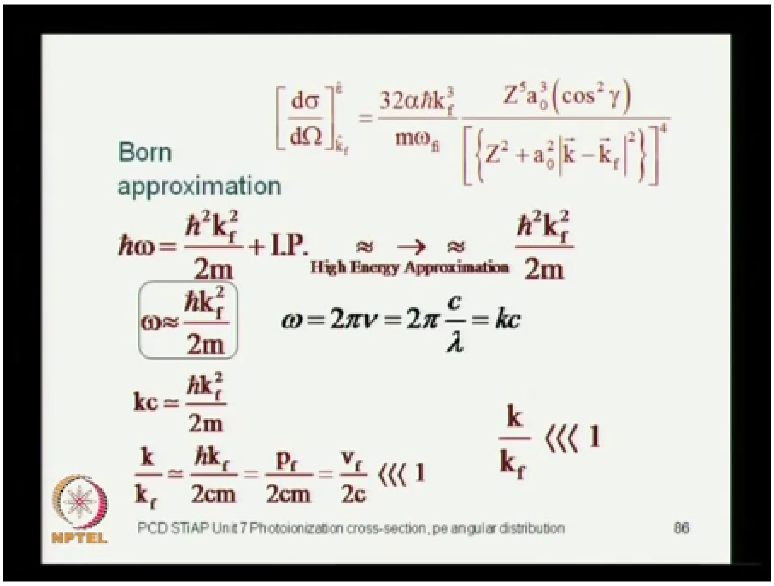

So, you have the forth power of this term in the denominator, and then we can develop and approximation, which is known as Born approximation, and in the Born approximation this expression gets a very simple form. Now, what is Born approximation, typically the Born approximation is employed, when you dealing with high energy processes, when you have a fairly large energy which is observed by the atom, and the electronic is knocked out.

So, when it comes out it has, so much of excess energy that it goes out very fast, and this is a nice case to consider, because if it is coming out very fast, then it is not going to have enough time to have co-relation with other electron to be expressed in the dynamical process. So, the independent particles approximation is also a good approximation, usually by large this is something which has to be qualified later, but by large the Born approximation is the good a approximation.

It justifies the independent partial approximation, you expected to work at high energies, because that is when the kinetic energy of this photo electron is much larger than the ionization potential. So, if the physical process is taking place for example, like a 1000 d v, and the binding energy is like it is of the order of 10 e v like 13.6 e v for the hydrogen atom. Then the kinetic energy with, which the electron comes out is much larger than the ionization potential, and this energy of the electromagnetic radiation is almost equal to the kinetic energy more or less given the fact that you are ignoring this small difference.

So, h cross omega in the born approximation is nearly equal to h cross square k f square by 2 m, which tells you if you cancel 1 power of h cross from both side, you have omega equal to h cross k square by 2 m. So, this is Born of approximation omega of course, is k time c, therefore, you have k time c, which is nearly equal to h cross k square by 2 m, and this tells you that k over k f will be equal to v f over twice c, c being the speed of light, which you know is huge. And in the Born approximation k over k f, then becomes a small quantity which in some of proximate expansion in skills you will be able to ignore, so this is the advantage of the born approximation that we will employ it.

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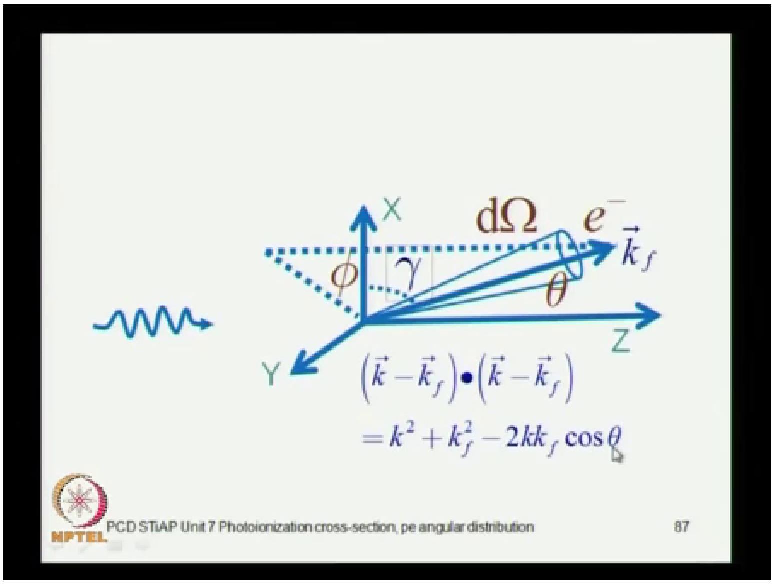

So, k over k f is most smaller than one, this is when the born approximation holes for the high energy processes, and the other quantity that we need is the square of the modules of k minus k f. So, that we will get by taking the scalar of product of these quantities, and you need again the cosine of the angle theta, theta is the angle between k and k f, which is the polar angle in our spherical in a polar co-ordinate system. K f is this k our choice of z axis is a long way incidents directions of electromagnetic radiation, so this is cosine theta this is the polar angle theta.

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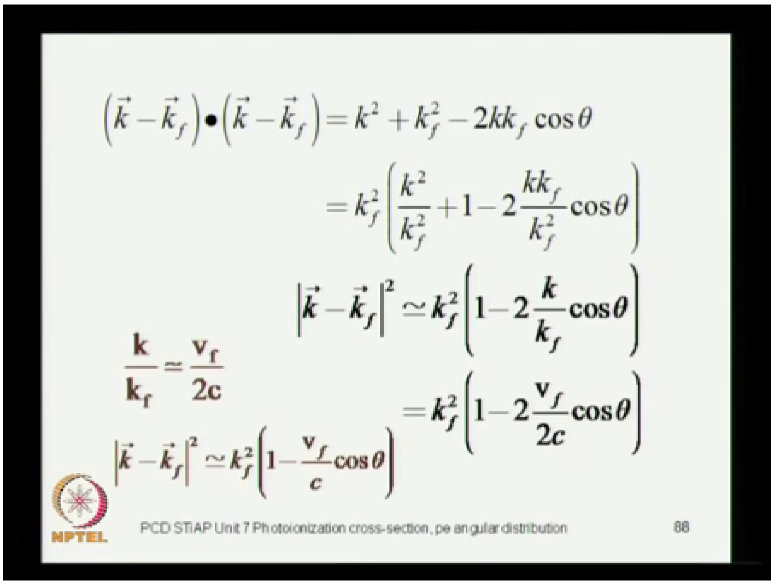

And you can now get k f square factor it out, because you have an approximation for k over k f, so it is good to factor out k f square, and where you have k over k f square you can make an approximation, which v f over 2 c which is the small quantity. So, you can ignore this term, and you have the rest of it, which is k f square times this becomes a gradable compare to 1. And then the rest of it is 1 minus v f over c times cosine theta, these are some other details Born approximation, and we can use this expression over here, where you need the modules square of k minus k f, which we have shown to be nearly equal to k f square.

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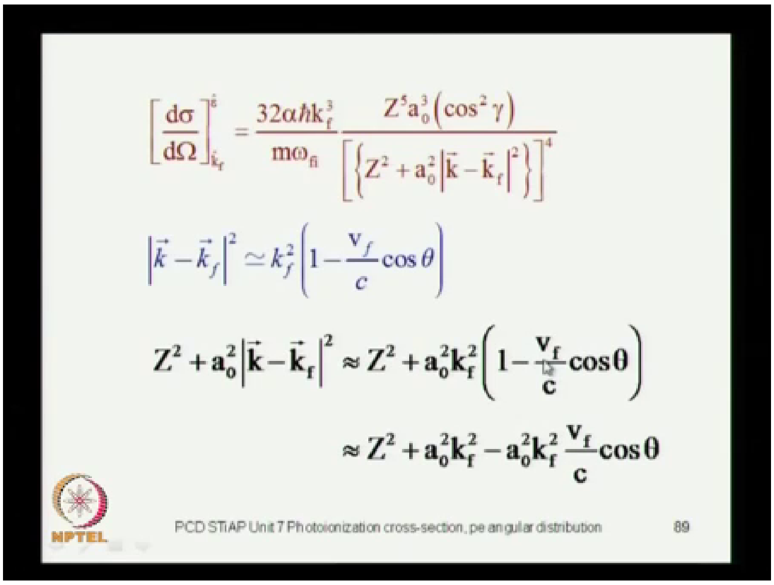

This nearly equal to is within the prime s of the Born approximation, and you have in the denominator z square plus a 0, square times, the square of this modules. The square of this modules is now written in terms of this square k f times this, so you have got 1 2 and 3 terms on the right side.

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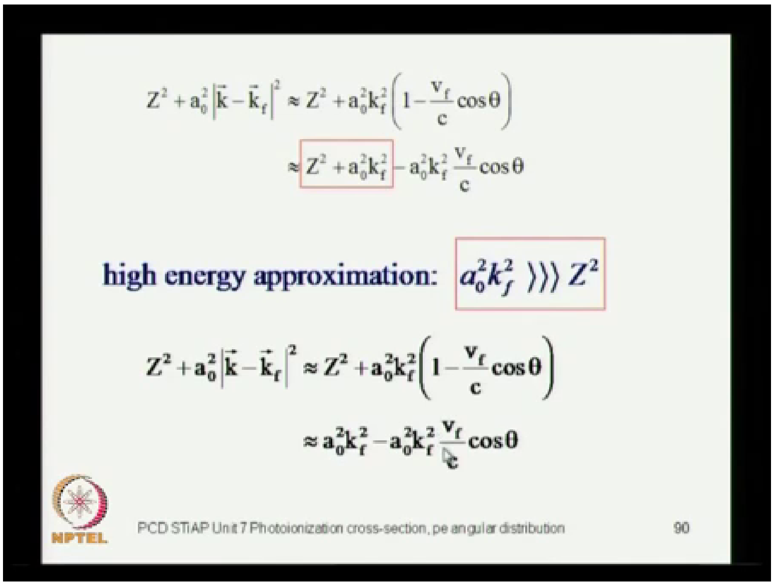

So, those are the three terms on the right side, but then this k f which is proportional momentum of the ejected electron, and this momentum is very high, because we are working within the prime s of the Born approximation. So, because this momentum is very high this term is much larger than z square, so you can ignore this z square compare to this, this is the high energy approximation that we are working with, this is the Born approximation.

And within this approximation this left hand side is nearly equal to this row right hand side, but this right hand side out of the 3 times, the first one drops. And you have the remaining 2 terms, which you can use in your expression for the differential cross section.

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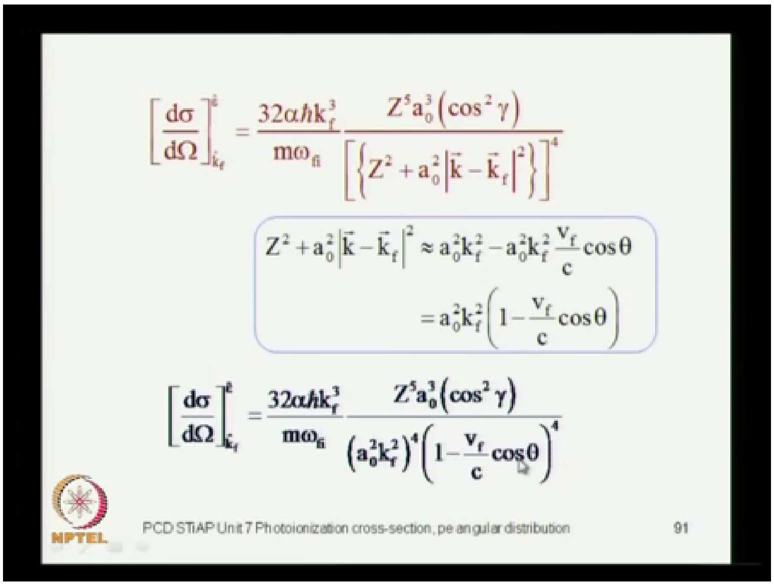

So, using that you have this a 0 square k f square, these are the remaining 2 terms, which will go over here, you had the thirty two alpha h cross k cube by m omega, coming from the previous expression from the different cross section. And now you have this 1 minus v over c cosine theta to the power 4, now this again you can explain and develop in approximation, because we over c is small.

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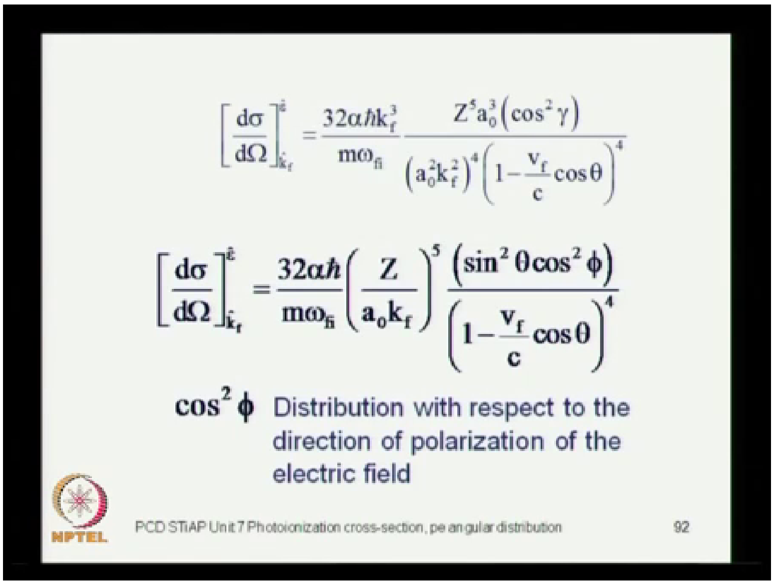

So, let us do that, so you got 1 minus v over c cosine theta to the power 4, you need the fourth power, you have got the cross square of gamma distribution, at this we have already seen equal to sin theta cosine phi, you have got the square of this. So, the differential cross section or unit solid angle in the given direction, for rejection has got this cos square phi distribution, in goes as the square of the cos sin of the as angle respect to the z explain.

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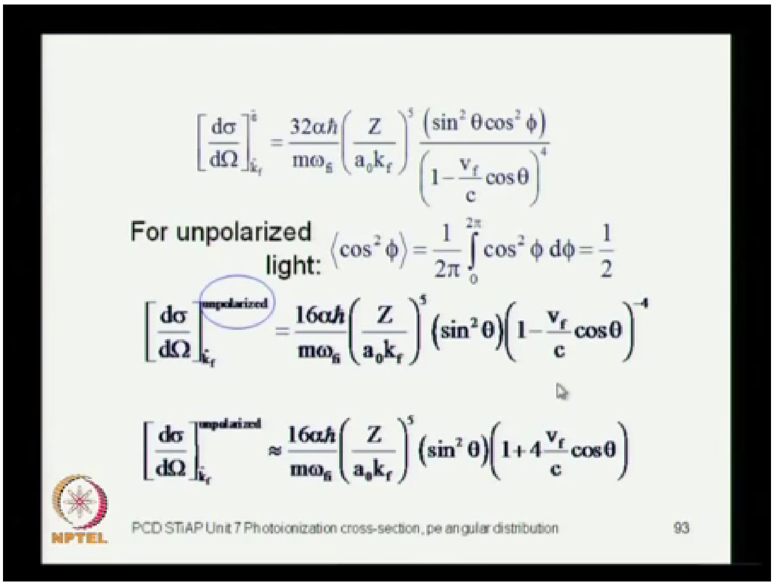

So, this is the extremely important result in photo ionization physics, now if you have the un-polarized light, so instead of this epsilon, you need to develop an expression for the un-polarized light. All have to you is do use average value of cos phi, because there as the angle will loss significance, so you need to use the average value of this cos square phi which is one half.

So, for un polarized light this expression for the differential cross section is half of this, so instead of 32 alpha, it cross you gets 60 alpha, 8 cross rest of expression is essentially the same. This is the expression for the un polarized light, and notice that you have got 1 minus v over c cos c that to the power 4 in the denominator. So, in the numerator it will come as one minus v over c cos theta at to the power minus 4, and if you expand it and take the leading term, you get 1 plus 4 times v over c cos theta, that is the leading term of their expansion.

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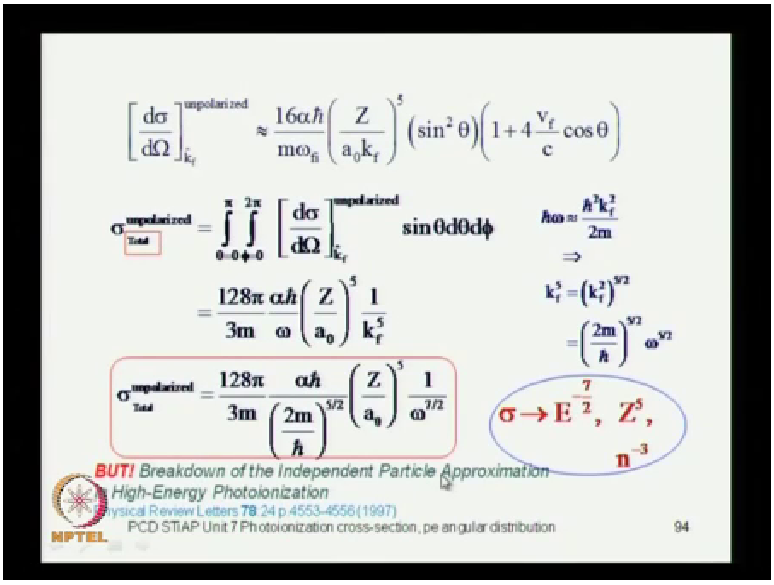

So, now, we almost have the final result, that the differential cross section is given by this one plus v over c cos theta, and now you can do an integration over angle, because this is the differential cross section at a given polar angle theta. What if you get the total cross section, that is to allow for photo exaction in all direction, and that will require you to integrate over going to 0 from pi and the entire solid angle.

So, when you carryout this integration there are two functions of theta over here, sin theta and there is the cos theta over here. So, when you this theta integration, this is the result that you get, it goes as z to the power 5, and a 0 to the power 5, you get 1 over k to the power 5, and what is k to the power 5 k to the power 5, you get in terms of energy, because energy is nearly equal to s square.

So, the fifth power of k will go as the 5 half power of frequency, because the second power of k goes as energy, so the fifth power of k goes as 5 half at power of frequency or energy. And one over k f cube goes as the denominator of this term on the right, and you get the expression for the total cross section for un polarized light, which goes as omega is here. There is omega to the power 5 half coming from this k f to the power 5, so omega to the power 5 half plus 1 power of omega will give you a power of 7 half in the denominator.

What it tells you is that the total cross section, is inversely proportional to the 7 half hour of the energy in the Born approximation, so this is an extremely important result it goes as e to the power minus 7 by 2, this is extremely important result in photo ionization physics. That if you want to have a first estimate of how will the photo ionization change with the energy, you know that it is going decrease with the energy, but at what rate does it decrease with energy.

So, it decreases at the rate of e to the power minus 7 by 2, it also goes as z to the power 5, so when you are doing hydrogenic atoms with large numbers of protons in the nuclease. It will go as z to the power 5, we have done this calculation just to illustrate for the hydrogen 1 s state, but you can do this for any other state of hydrogen atom. You can do the n l m, and you will require the corresponding for your transform, when you do it for an arbitrary quantum number, it will turn out and that something, which I am not going to illustrate over here.

But, I will use the result that, when you do it for arbitrary n, it goes as n t o the power minus 3, that does not come explicitly for the hydrogen 1 s, because n is equal to 1 in this case. So, this is a very important result, that the total photo ionization cross section for un polarized light goes e to the power minus 7 by 2, it goes z to the power 5, and n to the power minus 3. There is nevertheless a break down Born approximation, this is matter of detail one believes or one hopes that, this will always work at high energy.

But, then turn out there are write a detail co- relation, which really cannot be ignore even the born approximation. So, born approximation that you expect to whole very well in a at high energy, and you hope to use it in the independent particle approximation, we should which you hope will work in the born approximation, it really does not happen, because there are certain co relation which survive even at high energy. So, this is the matter of detail, but by large in excellent of approximation, and you can look up some of these details in literature.

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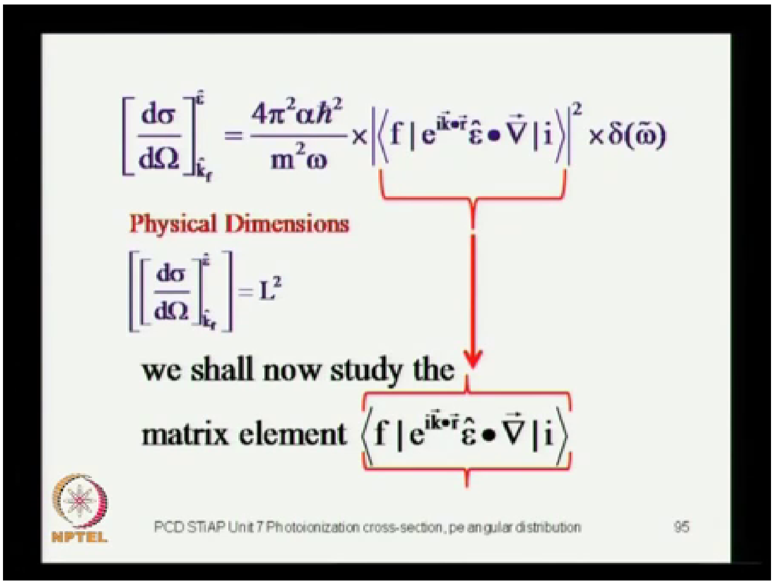

So, this is where I will conclude today's discussion, that you have the expression for the differential cross section, and we will then have to discuss some specific aspects of this matrix elements. And notice this matrix elements has got the gradient operator, it is the momentum operator, and then this form of the matrix element is some time call is the momentum form of the matrix elements. But, then you can also get what is called is the length of the matrix elements, so some of these details I will discuss in the next class.

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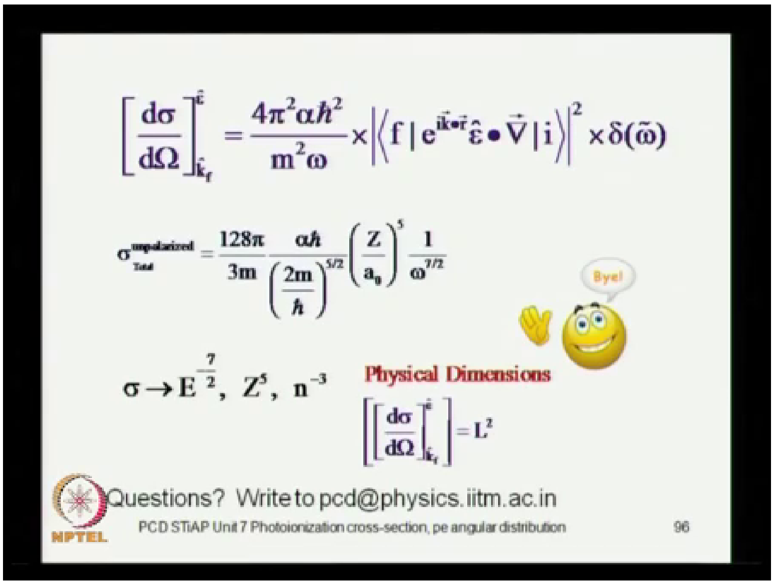

So, I will conclude today discussion over here, and we will discuss the length form in the momentum form of the matrix elements and the assaulters some rules and. So, on, so that would be the topic of discussion. So, the next class, but important thing over here is that the total cross section goes as energy to the minus 7 by 2, z to the 5 and n to the minus 3, so these are you know very important results photo ionization physics, there is any question I will be happy to take very well.

Thank you.