Select/Special Topics in Atomic Physics
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Lecture - 34
Atomic Photoionization Cross-Sections, Angular Distribution of Photoelectrons COOPER-ZARE Formula

Greetings, so today we will conclude unit 7 and this will be some sort of bridge class, which will invoke everything that we have learnt about photoionization including the boundary conditions. And then it will bridge this course work with some literature, so that you can read original literature in photoionization research. We will arrive at the COOPER ZARE formula for angular distribution of photoelectrons, I will not derive it in very great details, but I will certainly outline the essential pines, which lead us to, what is famously known as a COOPER ZARE formula for photoelectron angular distributions.

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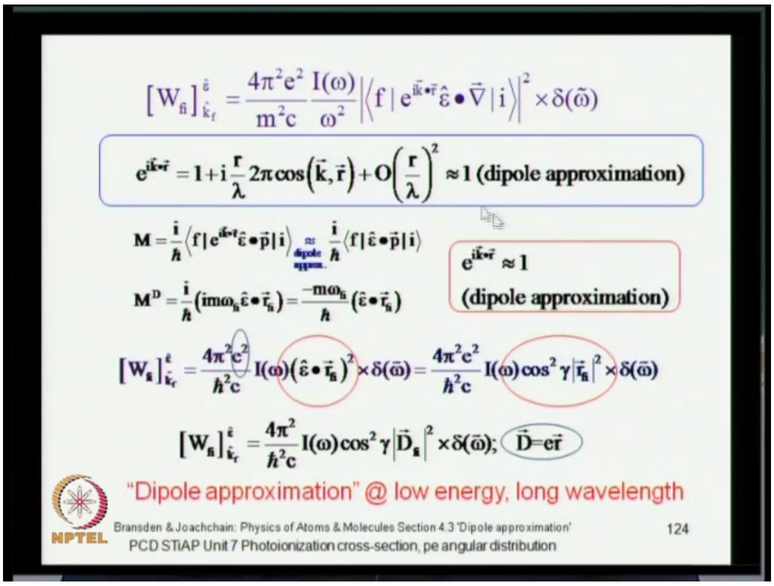

$$[W_{fi}]^{\hat{\varepsilon}}_{\hat{k}_f} = \frac{4\pi^2 e^2}{m^2 c}\frac{I(\omega)}{\omega^2}\left|\langle f|e^{i\vec{k}\bullet\vec{r}}\hat{\varepsilon}\bullet\vec{\nabla}|i\rangle\right|^2 \times \delta(\tilde{\omega})$$

$$e^{i\vec{k}\bullet\vec{r}} = 1 + i\frac{r}{\lambda}2\pi\cos(\vec{k},\vec{r}) + O\left(\frac{r}{\lambda}\right)^2 \approx 1 \text{ (dipole approximation)}$$

$$M = \frac{i}{\hbar}\langle f|e^{i\vec{k}\bullet\vec{r}}\hat{\varepsilon}\bullet\vec{p}|i\rangle \underset{\text{dipole approx.}}{\approx} \frac{i}{\hbar}\langle f|\hat{\varepsilon}\bullet\vec{p}|i\rangle$$

$$M^D = \frac{i}{\hbar}(im\omega_{fi}\hat{\varepsilon}\bullet\vec{r}_{fi}) = \frac{-m\omega_{fi}}{\hbar}(\hat{\varepsilon}\bullet\vec{r}_{fi})$$

$$e^{i\vec{k}\bullet\vec{r}} \approx 1 \text{ (dipole approximation)}$$

$$[W_{fi}]^{\hat{\varepsilon}}_{\hat{k}_f} = \frac{4\pi^2 e^2}{\hbar^2 c}I(\omega)(\hat{\varepsilon}\bullet\vec{r}_{fi})^2 \times \delta(\bar{\omega}) = \frac{4\pi^2 e^2}{\hbar^2 c}I(\omega)\cos^2\gamma|\vec{r}_{fi}|^2 \times \delta(\bar{\omega})$$

$$[W_{fi}]^{\hat{\varepsilon}}_{\hat{k}_f} = \frac{4\pi^2}{\hbar^2 c}I(\omega)\cos^2\gamma|\vec{D}_{fi}|^2 \times \delta(\bar{\omega}); \quad \vec{D} = e\vec{r}$$

"Dipole approximation" @ low energy, long wavelength

Bransden & Joachchain: Physics of Atoms & Molecules Section 4.3 'Dipole approximation'

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So, let us quickly recapitulate the relations that we have with us, so this is the expression for the photoionization rate. For photoionization process, in which a photoelectron is rejected along the unit vector k f and the electromagnetic radiation is considered to be polarized along the direction epsilon. And then we have this e to the i k dot r term in the expression for the matrix element, and if you take at a expansion of e to the i k dot r then you have higher order terms in r over lambda.

So, you can truncate this series for large wave length, so for large wave length, r over lambda will become a small quantity and higher powers of r over lambda can be ignored. And if you take the leading term, it is just e to the i k dot r equal to 1, which is known as the dipole approximation, in which case this matrix element of the gradient operator and this e to the i k dot r set equal to 1 gives you this relation in terms of the matrix element of the position operator.

We discussed in the previous class, how to connect the position operator, the matrix element of the position operator with matrix element of the momentum operator. So, these are related to each other in a certain approximate way means, depending on the potential being local and so on. So, these are some of the details that we discussed in the previous class, what you have in this rate expression is the modulus square. So, you get cos square gamma term here and then the square of the modulus of the matrix element of the position operator.

And to get there with this e square and this square of the matrix element of the position operator, you have got the matrix element of the dipole operator, which is why e to the i k dot r equal to 1 is refer to as the dipole approximation. Because, it is only when e to the i k dot r is set equal to 1, that you can develop the rest of the steps. So, this is the long wavelength approximation and it works reasonably well for 5 to 6000 electron volts above the ionization threshold, broadly speaking there are exceptions.

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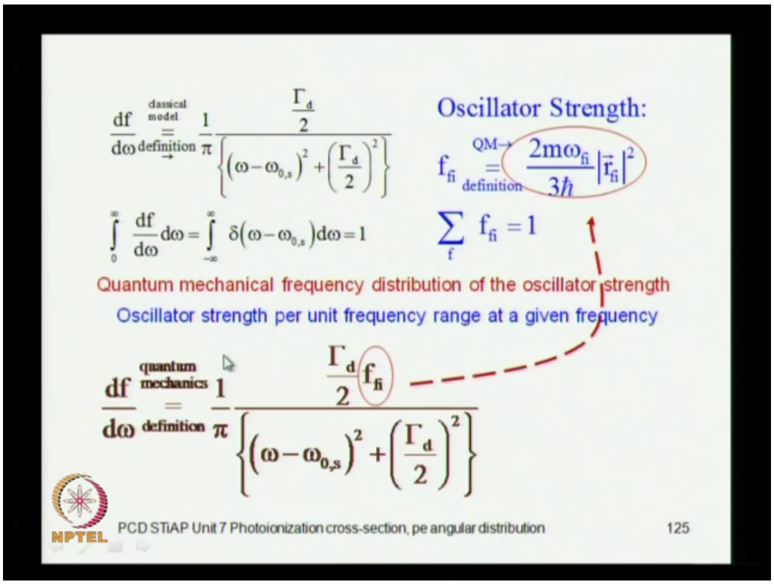

$$\frac{df}{d\omega} \underset{\substack{\text{definition}\\ \rightarrow}}{\overset{\substack{\text{classical}\\ \text{model}}}{=}} \frac{1}{\pi} \frac{\frac{\Gamma_d}{2}}{\left\{ \left(\omega - \omega_{0,s}\right)^2 + \left(\frac{\Gamma_d}{2}\right)^2 \right\}}$$

$$\int_0^\infty \frac{df}{d\omega} d\omega = \int_{-\infty}^\infty \delta\left(\omega - \omega_{0,s}\right) d\omega = 1$$

Oscillator Strength:

$$f_{fi} \underset{\text{definition}}{\overset{QM\rightarrow}{=}} \boxed{\frac{2m\omega_{fi}}{3\hbar} \left|\vec{r}_{fi}\right|^2}$$

$$\sum_f f_{fi} = 1$$

Quantum mechanical frequency distribution of the oscillator strength

Oscillator strength per unit frequency range at a given frequency

$$\frac{df}{d\omega} \underset{\text{definition}}{\overset{\substack{\text{quantum}\\ \text{mechanics}}}{=}} \frac{1}{\pi} \frac{\frac{\Gamma_d}{2} \boxed{f_{fi}}}{\left\{ \left(\omega - \omega_{0,s}\right)^2 + \left(\frac{\Gamma_d}{2}\right)^2 \right\}}$$

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And then we also introduced the oscillator strength, we introduce the quantum mechanical oscillators strength for transition from i to f. And then in the classical model of photoionization, we had the frequency distribution of the oscillator strength. So, there is a corresponding expression in quantum mechanics, which gives the oscillator strength per unit frequency and that is a very similar expression compared to the classical expression.

But, it incorporates this quantum mechanical expression for the matrix element of the position operator as well in the length form. So, this oscillator strength, this is in the quantum mechanical expression, so these two relations are combined and you get the quantum mechanical description of the oscillators strength, which is the oscillators strength per unit frequency. This is the frequency distribution of the oscillator strength or this is for a single transition.

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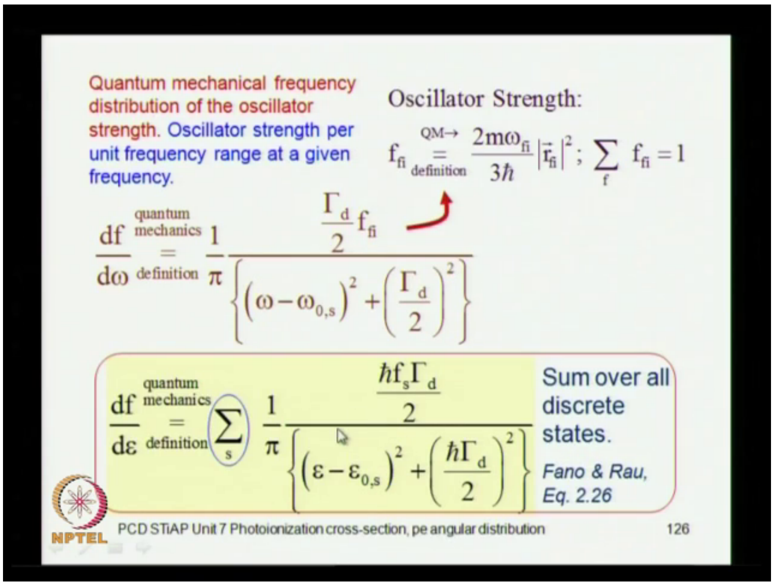

Quantum mechanical frequency distribution of the oscillator strength. Oscillator strength per unit frequency range at a given frequency.

Oscillator Strength:

$$f_{fi} \underset{\text{definition}}{\overset{\text{QM}\rightarrow}{=}} \frac{2m\omega_{fi}}{3\hbar}\left|\vec{r}_{fi}\right|^2; \sum_f f_{fi} = 1$$

$$\frac{df}{d\omega} \underset{\text{definition}}{\overset{\substack{\text{quantum}\\\text{mechanics}}}{=}} \frac{1}{\pi}\frac{\frac{\Gamma_d}{2} f_{fi}}{\left\{(\omega-\omega_{0,s})^2+\left(\frac{\Gamma_d}{2}\right)^2\right\}}$$

$$\frac{df}{d\varepsilon} \underset{\text{definition}}{\overset{\substack{\text{quantum}\\\text{mechanics}}}{=}} \sum_s \frac{1}{\pi}\frac{\frac{\hbar f_s \Gamma_d}{2}}{\left\{(\varepsilon-\varepsilon_{0,s})^2+\left(\frac{\hbar\Gamma_d}{2}\right)^2\right\}}$$

Sum over all discrete states.

Fano & Rau, Eq. 2.26

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But then you need to sum over all the transition, so there is a summation over all possible discrete states, which you incorporate and you will find an extension discussion on this in Fano and Rau’s book. So, this is the quantum mechanical description of the oscillators strength and it has been so defined such that, you can carry out certain extrapolations of very important dynamical properties across the ionization threshold, when you go from discrete to the continuum.

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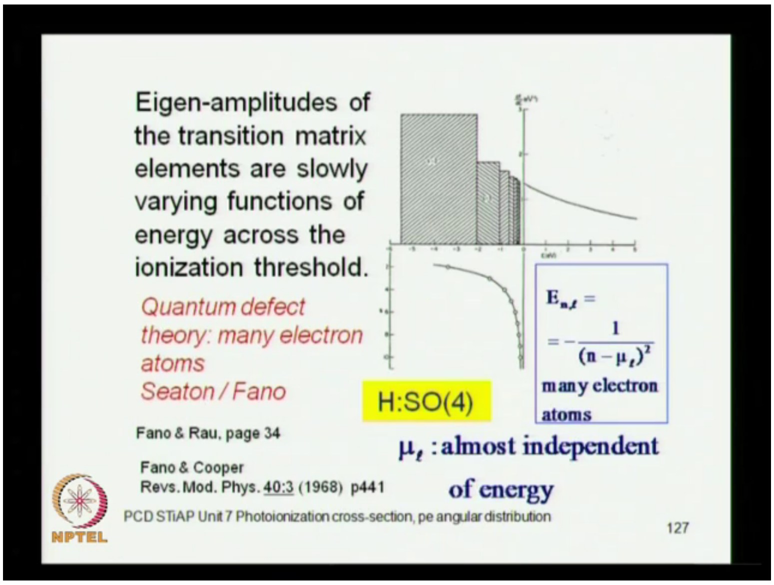

Eigen-amplitudes of the transition matrix elements are slowly varying functions of energy across the ionization threshold.

Quantum defect theory: many electron atoms
Seaton / Fano

Fano & Rau, page 34

Fano & Cooper
Revs. Mod. Phys. 40:3 (1968) p441

H:SO(4)

$E_{n\ell} = -\frac{1}{(n-\mu_\ell)^2}$ many electron atoms

μ_ℓ : almost independent of energy

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And I will draw your attention to this figure from Fano and Cooper's review of review, which appeared in reviews of model physics and this is available also in Fano and Rau's book. And this is an oscillator strength distribution, so you have got the discrete part on the left of this vertical line, so this is the discrete part. And on the right side is the continuum part and you have plotted in this the oscillators strength distribution, which has been defined according to the prescription.

And there is a certain normalization procedure and I will not going to those details, but just draw your attention to this. What it allows you to do, is to find that there is a continuity you notice that, if you extrapolate this curve, you have a certain continuity, which allows you to get property, to connect properties in the discrete part of the spectrum to properties in the continuum. And in particular, what are call this Eigen amplitudes of the transition matrix elements, these are slowly varying functions of energy across the ionization threshold.

So, the ionization threshold is over here and over here if you take a very small energy region delta e near the ionization threshold, in this region the matrix element is almost independent of energy rate, is hardly changing with respect to energy. And this allows you to study, to connect properties of the discrete spectrum with properties in the continuum. And there is a good bit of work, which has been done by Seaton and Fano and this takes has to, what is known as the quantum defect theory, which is applicable from any electron atoms.

Here, I have shown this spectrum for the hydrogen atom, which is the single electron atoms but then it is utility and it is power is most exploited for many electron systems, for which we do not exact solutions. And then you develop approximation methods and quantum defect method is one of the approximation methods, which gives us great, an excellent handle on this.

What it also does is that, it expresses energy not just as a function of n, which is the case for the hydrogen atom, according to the which has got the SO 4 symmetry, but other atoms will not have the SO symmetry when you have more than one electron. And then the 1 over n square formula has to be corrected by 1 minus 1 upon n minus mu whole square and mu depends on l, so the energy depends both on n as well as l. So, mu is what is called as quantum defect and all these goes into the formulation of the quantum defect theory developed by Seaton and Fano.

And as a matter of fact, there is the huge of number of references an atomic physics to Fano's work and the number of citations to Fano work in fact, exceeds the number of citations to some very famous papers including by a Niels Bohr's, Schrodinger's and so on. So, this is one of the classic works in quantum mechanics and atomic physics, which is the great importance. So, it is good to get introduced to that.

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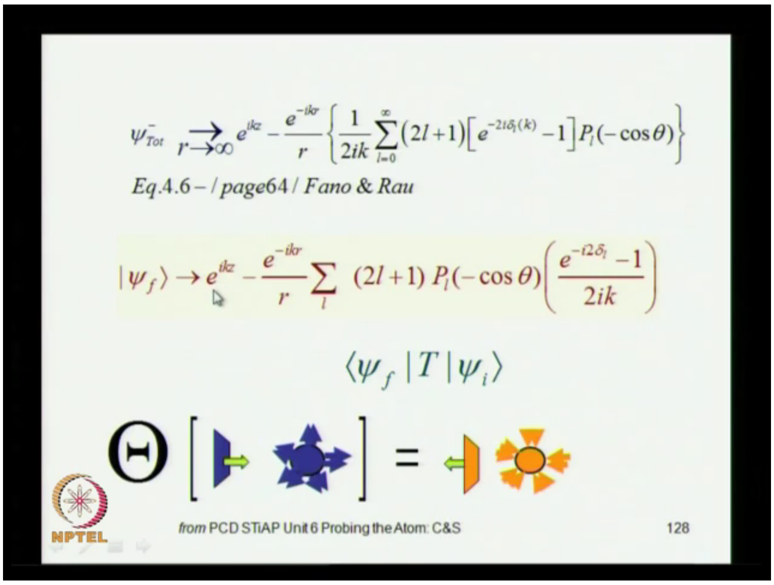

$$\psi^{-}_{Tot} \xrightarrow[r\to\infty]{} e^{ikz} - \frac{e^{-ikr}}{r}\left\{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{-2i\delta_l(k)}-1\right]P_l(-\cos\theta)\right\}$$

Eq.4.6 – / page64 / Fano & Rau

$$|\psi_f\rangle \to e^{ikz} - \frac{e^{-ikr}}{r}\sum_{l}(2l+1)\,P_l(-\cos\theta)\left(\frac{e^{-i2\delta_l}-1}{2ik}\right)$$

$$\langle\psi_f|T|\psi_i\rangle$$

$$\Theta\,[\quad] = $$

from PCD STiAP Unit 6 Probing the Atom: C&S

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So, our interest is in determining this matrix element, this is the matrix element for transition from an initial state to of final state. We are studying photo ionization, but we are going to use techniques from quantum collision physics and we known that, the solutions of quantum collision physics and photo ionization at connected to each other, prove time reversal symmetry, which we studied in the unit 6. So, we will use this relationship of getting the final state wave function according to the ingoing wave boundary conditions, which we studied in the previous unit.

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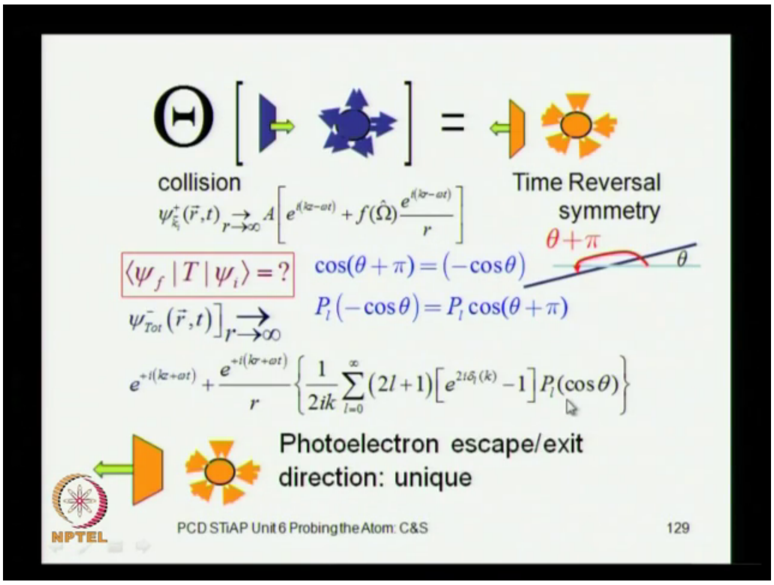

$$\Theta \left[\quad \right] =$$

collision

$$\psi^{+}_{\vec{k}_i}(\vec{r},t) \xrightarrow[r\to\infty]{} A\left[e^{i(kz-\omega t)} + f(\hat{\Omega})\frac{e^{i(kr-\omega t)}}{r} \right]$$

Time Reversal symmetry

$$\boxed{\langle \psi_f | T | \psi_i \rangle = ?}$$

$$\cos(\theta+\pi) = (-\cos\theta)$$

$$P_l(-\cos\theta) = P_l\cos(\theta+\pi)$$

$$\psi^{-}_{Tot}(\vec{r},t)\Big]_{r\to\infty} \rightarrow$$

$$e^{+i(kz+\omega t)} + \frac{e^{+i(kr+\omega t)}}{r}\left\{ \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta) \right\}$$

Photoelectron escape/exit direction: unique

PCD STiAP Unit 6 Probing the Atom: C&S

And the advantages of this is, that we have seen that in the photoelectric effect, when you have the electron ejected, that is the only direction with reference to which you can measure different angle. Because, that is the unique direction, there is no electron in the initial state in the photoionization process. The initial state consist of a photon and an atom, it is a final state which has got and ion and an electron, which is similar to the final state of electron ion scattering.

So, in the initial state, there is no electron direction to reference to, what you have is the photoelectron escape direction, which is a unique channel. And this is the direction with reference to which, angles will be measured and the two processes are connected to each other through the time reversal symmetry as we have learned.

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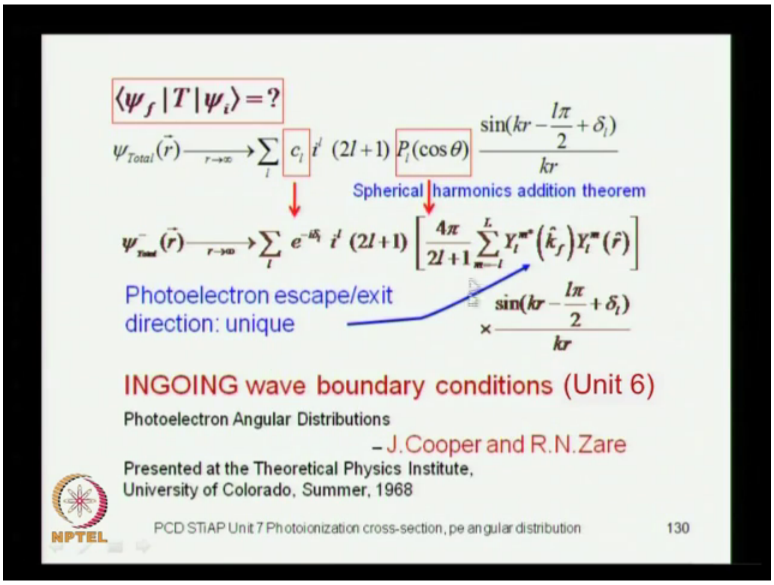

$$\boxed{\langle \psi_f | T | \psi_i \rangle = ?}$$

$$\psi_{Total}(\vec{r}) \xrightarrow[r\to\infty]{} \sum_l \boxed{c_l}\, i^l\, (2l+1)\, \boxed{P_l(\cos\theta)}\, \frac{\sin(kr - \frac{l\pi}{2} + \delta_l)}{kr}$$

Spherical harmonics addition theorem

$$\psi^-_{Total}(\vec{r}) \xrightarrow[r\to\infty]{} \sum_l e^{-i\delta_l}\, i^l\, (2l+1) \left[\frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_l^{m*}(\hat{k}_f) Y_l^m(\hat{r})\right] \times \frac{\sin(kr - \frac{l\pi}{2} + \delta_l)}{kr}$$

Photoelectron escape/exit direction: unique

INGOING wave boundary conditions (Unit 6)

Photoelectron Angular Distributions

– J.Cooper and R.N.Zare

Presented at the Theoretical Physics Institute,
University of Colorado, Summer, 1968

So, we will use that in writing our expression for the total wave function c l, this is an expansion in terms of the angle of functions at the radial functions. But then the expansion coefficient c l of these partial waves must be chosen according to the boundary conditions. At the boundary condition of relevance over here, is the ingoing wave boundary condition. And what is that c l must be given by e to the minus i delta l, that is the boundary condition that we discussed in unit 6.

So, c l is given by e to the minus i delta l, here by making use of this spherical harmonics addition theorem, you can expand this in terms of this m going from minus l to plus l and this is was done in unit 6. So, this is what will lead us to the COOPER ZARE formula, this expression using the ingoing wave boundary condition.

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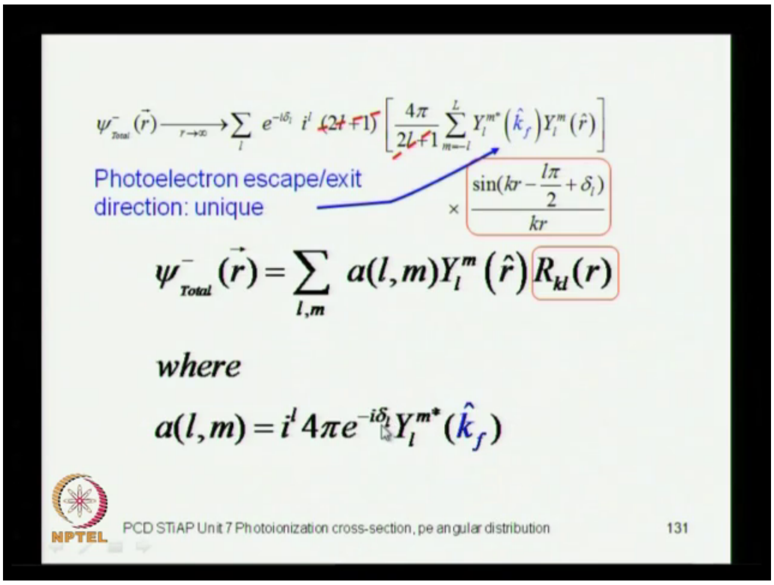

$$\psi^{-}_{Total}(\vec{r}) \xrightarrow[r\to\infty]{} \sum_{l} e^{-i\delta_l}\, i^{l}\, \cancel{(2l+1)} \left[\frac{4\pi}{\cancel{2l+1}} \sum_{m=-l}^{L} Y_l^{m*}\left(\hat{k}_f\right) Y_l^{m}(\hat{r})\right] \times \boxed{\frac{\sin(kr - \frac{l\pi}{2} + \delta_l)}{kr}}$$

Photoelectron escape/exit direction: unique

$$\psi^{-}_{Total}(\vec{r}) = \sum_{l,m} a(l,m) Y_l^{m}\left(\hat{r}\right) \boxed{R_{kl}(r)}$$

where

$$a(l,m) = i^{l} 4\pi e^{-i\delta_l} Y_l^{m*}(\hat{k}_f)$$

So, let us have a look at this, so here you find that the 12 plus 1 and this 12 plus 1 will cancel each other. I have use the spherical harmonic addition theorem to expand the p l cos theta, so the 12 plus 1 in the enumerator and the denominator cancel each other. And you can write this total wave function according to the ingoing wave boundary condition in terms of this radial function, which is this, which includes the scattering phase shift. This is written as R, radial function R of r then there is spherical harmonic Y l m of r, which is coming from here.

And then everything else which includes this i to the l and e to the minus i delta l, the phase shift, this factor 4 pi and the spherical harmonic corresponding to the direction of the photoelectron escape direction, which is the unique direction. That goes into an angle of factor, which is written compactly as a l m, because it will depend on l and the dependence includes the dependence of the phase shift delta on l. It will also parametrically depend on the energy, because of phase shift depends on energy.

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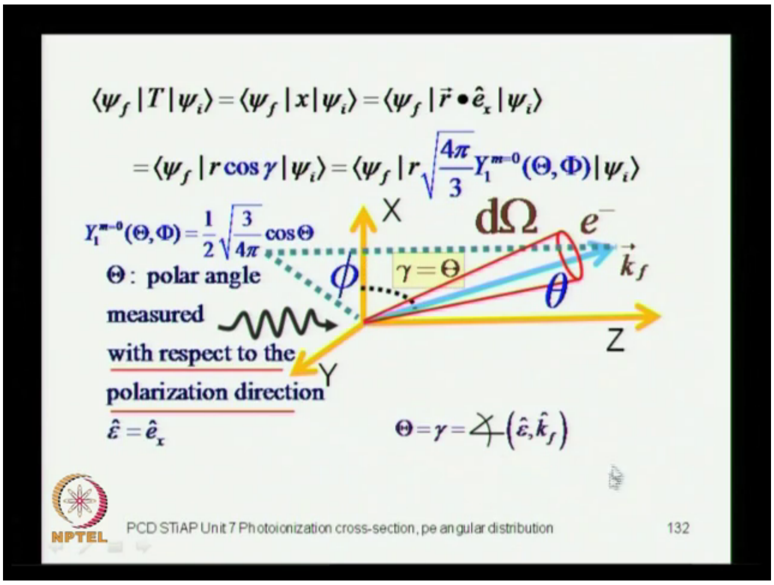

$$\langle\psi_f|T|\psi_i\rangle=\langle\psi_f|x|\psi_i\rangle=\langle\psi_f|\vec{r}\bullet\hat{e}_x|\psi_i\rangle$$

$$=\langle\psi_f|r\cos\gamma|\psi_i\rangle=\langle\psi_f|r\sqrt{\frac{4\pi}{3}}Y_1^{m=0}(\Theta,\Phi)|\psi_i\rangle$$

$$Y_1^{m=0}(\Theta,\Phi)=\frac{1}{2}\sqrt{\frac{3}{4\pi}}\cos\Theta$$

Θ: polar angle measured with respect to the polarization direction

$\hat{\varepsilon}=\hat{e}_x$

$$\Theta=\gamma=\measuredangle\left(\hat{\varepsilon},\hat{k}_f\right)$$

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So, this is what you want to determine, this is the matrix element and you want to determine the matrix element of the position operator. So, we take the r dot e x, e x is the direction of polarization and this angle is cosine gamma. So, this is the gamma, which is the angle between the polarization direction, which is along e x and the photoelectron escape direction. So, this is like measuring a polar angle, not with respect to Z axis of here, but with respect to the direction of polarization.

So, theta, this is an uppercase theta as opposed to this theta, so there are two theta angles, this theta angle is a polar angle with respect to the Z axis, as we typically use is spherical polar coordinate system. This is a different theta, which is like the uppercase theta and this is the polar angle measured with respect to the polarization direction which is epsilon, which is along the X axis, which is along the e x unit vector. So, theta is this angle between epsilon and this direction of polarization and the photoelectron escape direction, so this is the angle that is of importance in the present context.

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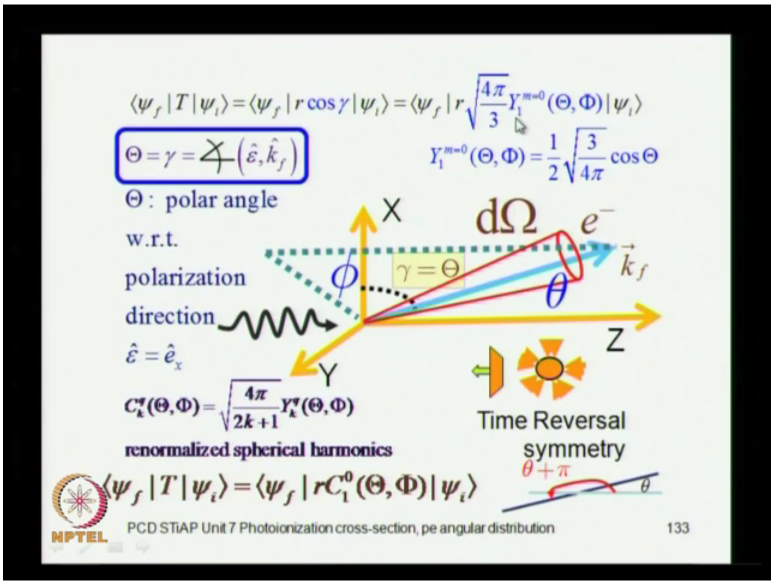

$$\langle \psi_f | T | \psi_i \rangle = \langle \psi_f | r\cos\gamma | \psi_i \rangle = \langle \psi_f | r\sqrt{\frac{4\pi}{3}} Y_1^{m=0}(\Theta,\Phi) | \psi_i \rangle$$

$$\boxed{\Theta = \gamma = \measuredangle(\hat{\varepsilon}, \hat{k}_f)}$$

$$Y_1^{m=0}(\Theta,\Phi) = \frac{1}{2}\sqrt{\frac{3}{4\pi}}\cos\Theta$$

Θ : polar angle w.r.t. polarization direction $\hat{\varepsilon} = \hat{e}_x$

$$C_k^q(\Theta,\Phi) = \sqrt{\frac{4\pi}{2k+1}} Y_k^q(\Theta,\Phi)$$

renormalized spherical harmonics

$$\langle \psi_f | T | \psi_i \rangle = \langle \psi_f | r C_1^0(\Theta,\Phi) | \psi_i \rangle$$

Time Reversal symmetry

So, this cosine gamma is a spherical harmonics for l equal to 1, m equal to 0, you can always write it like that. And this is the direction with respect to which, you are measuring the angles and it is useful to introduce what are called as renormalized spherical harmonics. They are same as spherical harmonics as you can see, there is just a constant factor root of 4 pi over 2 k plus 1, which is like normalization, which is called as renormalization of the spherical harmonics.

So, it is just the size which is scaled by this root of 4 pi over 2 k plus 1 and this matrix element is therefore, written in terms of the matrix element of the renormalized spherical harmonics. So, there is a factor of r over here and there is the rest of the spherical harmonics and then there is this root of 4 pi over 3, so that is already contained over here. So, you can write this as the matrix element of the renormalized spherical harmonics, so that is for k in this case, which is Y 1, so k is equal to 1. So, you have 2 plus 3 in the denominator, it is root 4 pi over 3 as you get it.

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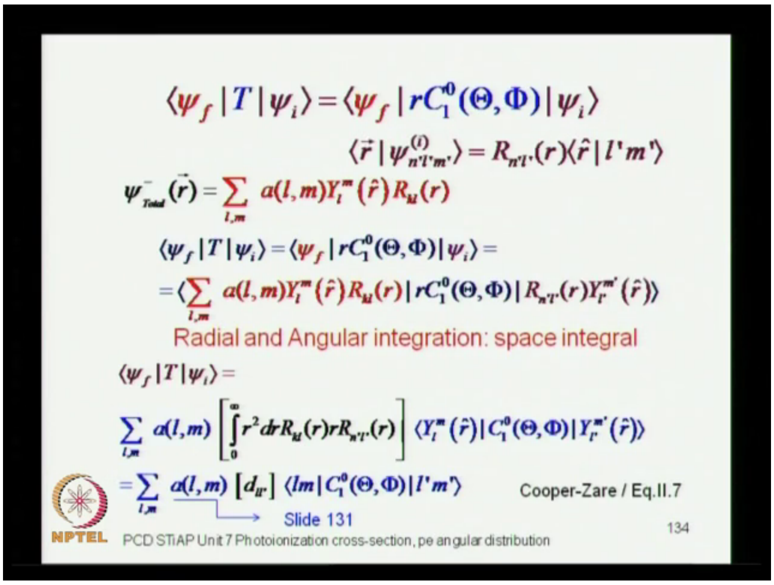

$$\langle \psi_f | T | \psi_i \rangle = \langle \psi_f | r C_1^0(\Theta,\Phi) | \psi_i \rangle$$

$$\langle \vec{r} | \psi^{(i)}_{n'l'm'} \rangle = R_{n'l'}(r) \langle \hat{r} | l'm' \rangle$$

$$\psi^-_{Total}(\vec{r}) = \sum_{l,m} a(l,m) Y_l^m(\hat{r}) R_{kl}(r)$$

$$\langle \psi_f | T | \psi_i \rangle = \langle \psi_f | r C_1^0(\Theta,\Phi) | \psi_i \rangle =$$

$$= \langle \sum_{l,m} a(l,m) Y_l^m(\hat{r}) R_{kl}(r) | r C_1^0(\Theta,\Phi) | R_{n'l'}(r) Y_{l'}^{m'}(\hat{r}) \rangle$$

Radial and Angular integration: space integral

$$\langle \psi_f | T | \psi_i \rangle =$$

$$\sum_{l,m} a(l,m) \left[\int_0^\infty r^2 dr R_{kl}(r) r R_{n'l'}(r) \right] \langle Y_l^m(\hat{r}) | C_1^0(\Theta,\Phi) | Y_{l'}^{m'}(\hat{r}) \rangle$$

$$= \sum_{l,m} \underbrace{a(l,m)}_{\to \text{Slide 131}} [d_{ll'}] \langle lm | C_1^0(\Theta,\Phi) | l'm' \rangle$$

Cooper-Zare / Eq.II.7

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So, this is the matrix element of the renormalized spherical harmonics and now, you have the matrix element of this r into C in an initial state, which is hydrogenic. So, we are using the non relativistic formulation at this point, so this will be n l and m, so I am using n prime, l prime and m prime for the initial state. So, this is the wave function for the hydrogenic initial state, the final state wave function we have written in terms of this expansion, which we have just discussed.

So now, you plugin this matrix element, sandwich it between these final state and the initial state. So, this is the final state, this is the initial state, you got a summation over l and m and this is essentially, what is this, this is the space integral. This matrix element is essentially space integral and it includes integration over r going from 0 to infinity and also integration over the angles theta and pi, which will go over the entire space. So, this is radial integral, so this is an integration from 0 to infinity of r square d r is the volume element.

You have got the radial function of the initial state, initial bounds state, this is the continuum state radial function, which includes the phase shift, was argument includes the phase shift. This is the operator r, which is coming in from here, this is the matrix element of r into C, so this r comes in over here. So, this is the radial integral and then there is an angular integration, which is the matrix element of the renormalized spherical harmonics between the angular functions of the final state, for which you have got the Y l m of r and the Y l m prime of r.

The rest of the angle of factors are contained in the a l m, so this is the angular integration, which is to be determined. So, there is one angular integration over here and the space integration over here then multiplication scaled by this factor a l m and then you need to some over l and m. So, that is the matrix element, that you will have to put and that will give you the transition rate and then it is modulus square will give you the transition probability, which we have related to the photo ionization cross sections so that, you will get the complete distribution. But then it will also be connected to the d sigma by d omega, which is the angle dependent cross section. So, it is the differential cross section for units solid angle, so a l m, we have already defined earlier on the slide 131, we will use that from there.

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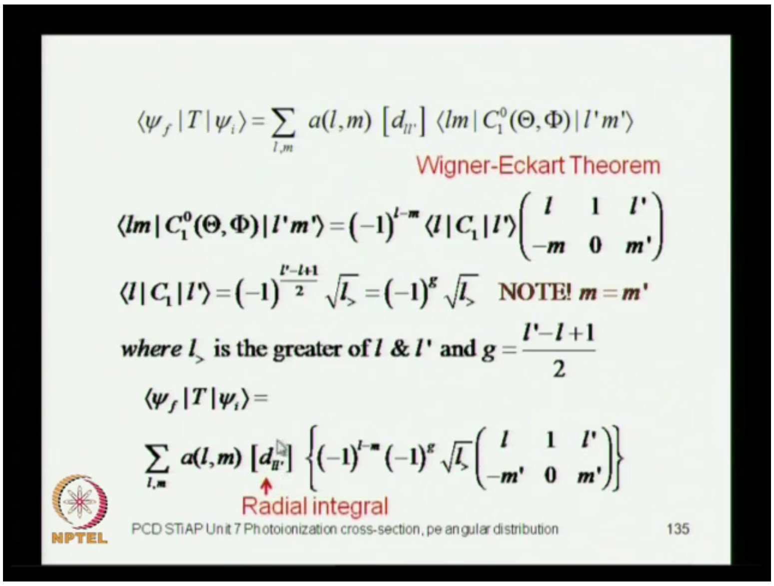

$$\langle \psi_f | T | \psi_i \rangle = \sum_{l,m} a(l,m)\,[d_{ll'}]\,\langle lm | C_1^0(\Theta,\Phi) | l'm' \rangle$$

Wigner-Eckart Theorem

$$\langle lm | C_1^0(\Theta,\Phi) | l'm' \rangle = (-1)^{l-m} \langle l \| C_1 \| l' \rangle \begin{pmatrix} l & 1 & l' \\ -m & 0 & m' \end{pmatrix}$$

$$\langle l \| C_1 \| l' \rangle = (-1)^{\frac{l'-l+1}{2}} \sqrt{l_>} = (-1)^g \sqrt{l_>} \quad \text{NOTE! } m = m'$$

where $l_>$ is the greater of l & l' and $g = \dfrac{l'-l+1}{2}$

$$\langle \psi_f | T | \psi_i \rangle =$$

$$\sum_{l,m} a(l,m)\,[d_{ll'}] \left\{ (-1)^{l-m} (-1)^g \sqrt{l_>} \begin{pmatrix} l & 1 & l' \\ -m' & 0 & m' \end{pmatrix} \right\}$$

↑ Radial integral

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And now, we need the matrix element of this renormalized spherical harmonics and to get this, we use the Wigner Eckart theorem. And that will give factor of all the matrix element of C 1 and it will give us Clebsch Gordon coefficient or a Wigner 3 j symbol, they are all related to each other. So, I will let you work with the details and using the Wigner Eckart theorem, you get this expression. So now, the angular part and the space part and the physical part is already taken care of.

And this particular matrix element of the reduce spherical harmonics from elementary angle of momentum algebra is given by this space factor time square root of l large, where l large is the larger of l and l prime, and g is given by this l prime minus l plus 1 by 2. So, this is what you get and once you put in all of these expressions, you get the matrix element in terms of this angular factors including the Wigner 3 j symbol, which is essentially Clebsch Gordon coefficient and then you have got the radial integral over here, so we will have to use the radial integral explicitly.

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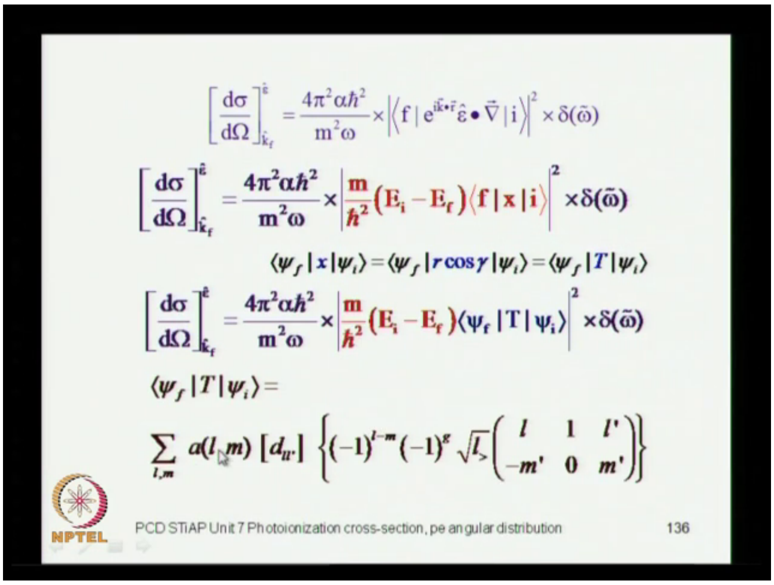

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{\varepsilon}} = \frac{4\pi^2\alpha\hbar^2}{m^2\omega} \times \left|\langle f | e^{i\vec{k}\cdot\vec{r}}\hat{\varepsilon}\bullet\vec{\nabla} | i\rangle\right|^2 \times \delta(\tilde{\omega})$$

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{\varepsilon}} = \frac{4\pi^2\alpha\hbar^2}{m^2\omega} \times \left|\frac{m}{\hbar^2}(E_i - E_f)\langle f | x | i\rangle\right|^2 \times \delta(\tilde{\omega})$$

$$\langle\psi_f | x | \psi_i\rangle = \langle\psi_f | r\cos\gamma | \psi_i\rangle = \langle\psi_f | T | \psi_i\rangle$$

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{\varepsilon}} = \frac{4\pi^2\alpha\hbar^2}{m^2\omega} \times \left|\frac{m}{\hbar^2}(E_i - E_f)\langle\psi_f | T | \psi_i\rangle\right|^2 \times \delta(\tilde{\omega})$$

$$\langle\psi_f | T | \psi_i\rangle =$$

$$\sum_{l,m} a(l,m)\,[d_{ll'}]\left\{(-1)^{l-m}(-1)^g\sqrt{l_>}\begin{pmatrix} l & 1 & l' \\ -m' & 0 & m' \end{pmatrix}\right\}$$

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And we are now going to plug it back into the expression for the differential cross section, which was essentially the matrix element of this operator, the gradient operator. And then in the dipole approximation, you get the connection between the momentum and the position operator, so that is all coming together now. And all of these relations are going to come together, because we are now looking at the matrix element of the position operator, the x operator, which is r cosine gamma, which is the matrix element of this T.

But then psi f is to be used according to the ingoing wave boundary condition, as we have just discussed. And we will of course, need the modulus square of this and this matrix element is now includes these angular factors, the Wigner 3 j or the Clebsch Gordon coefficient as we have. These radial integrals, these angle of factors and the summation over l and m and l of course, goes from 0 through infinity. However, you do not need these infinite summations, because you are working within the dipole approximation. So, transitions only to delta l equal to plus or minus 1 will be involved, so you will have to deal with fewer terms.

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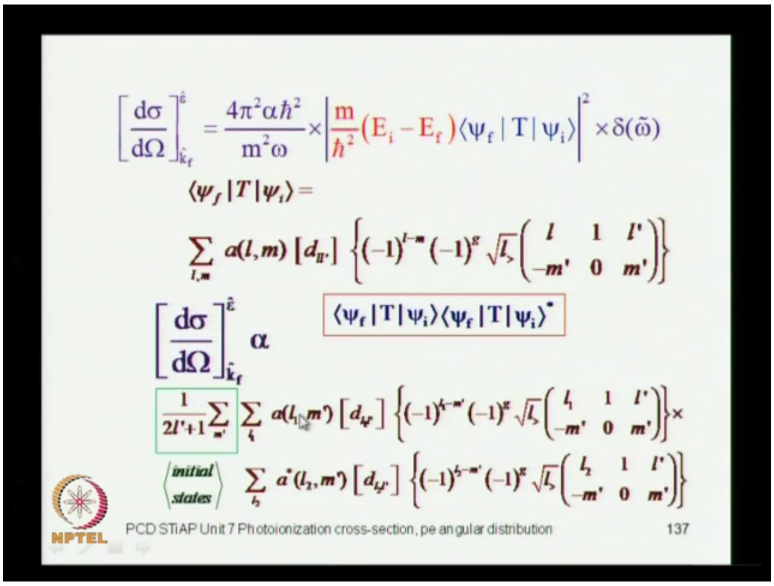

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{\varepsilon}} = \frac{4\pi^2\alpha\hbar^2}{m^2\omega} \times \left|\frac{m}{\hbar^2}(E_i - E_f)\langle\psi_f|T|\psi_i\rangle\right|^2 \times \delta(\tilde{\omega})$$

$$\langle\psi_f|T|\psi_i\rangle =$$

$$\sum_{l,m} a(l,m)\,[d_{ll'}]\left\{(-1)^{l-m}(-1)^{g}\sqrt{l_>}\begin{pmatrix} l & 1 & l' \\ -m' & 0 & m' \end{pmatrix}\right\}$$

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{\varepsilon}} \alpha \qquad \boxed{\langle\psi_f|T|\psi_i\rangle\langle\psi_f|T|\psi_i\rangle^*}$$

$$\boxed{\frac{1}{2l'+1}\sum_{m'}} \sum_{l_1} a(l_1,m')\,[d_{l_1l'}]\left\{(-1)^{l_1-m'}(-1)^{g}\sqrt{l_>}\begin{pmatrix} l_1 & 1 & l' \\ -m' & 0 & m' \end{pmatrix}\right\}\times$$

$$\left\langle \begin{matrix} \text{initial} \\ \text{states} \end{matrix} \right\rangle \sum_{l_2} a^*(l_2,m')\,[d_{l_2l'}]\left\{(-1)^{l_2-m'}(-1)^{g}\sqrt{l_>}\begin{pmatrix} l_2 & 1 & l' \\ -m' & 0 & m' \end{pmatrix}\right\}$$

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And then when you take the modulus square, you have the psi f T psi i and then the complex conjugate of that, so this is the modulus square that you are going to need. So, we have this expression for the matrix element of the operator T and you will need the complex conjugate of that, to multiply this. So, you will have a summation over l in one of these expressions and again a summation over l and m in the complex conjugate. So, you will have summations over l 1 and l 2, there are two summations over l quantum numbers and two summations over m quantum numbers.

You will of course, exploit the orthogonality relations of the Clebsch Gordon coefficients, so you are then left with an averaging over all the m prime stage, because m prime goes from minus l to plus m. So, there was a division by 1 over 2 l plus 1 when you average out overall those states, so you got 1 over 2 l plus 1 factor and you now have a relation, which has got a quadratic term in the radial integral. This is the radial integral d, it comes twice, once from here and the other from here, so there is no complex conjugation, because the radial integrals are real.

And then you have got two of these 3 js and the corresponding phase factors and the square root of the orbital angular momentum quantum number. And then two of these a factors, the angle of factors a l m, one coming from this element and the complex conjugate coming from here, so those are all the terms, so everything is taken care of.

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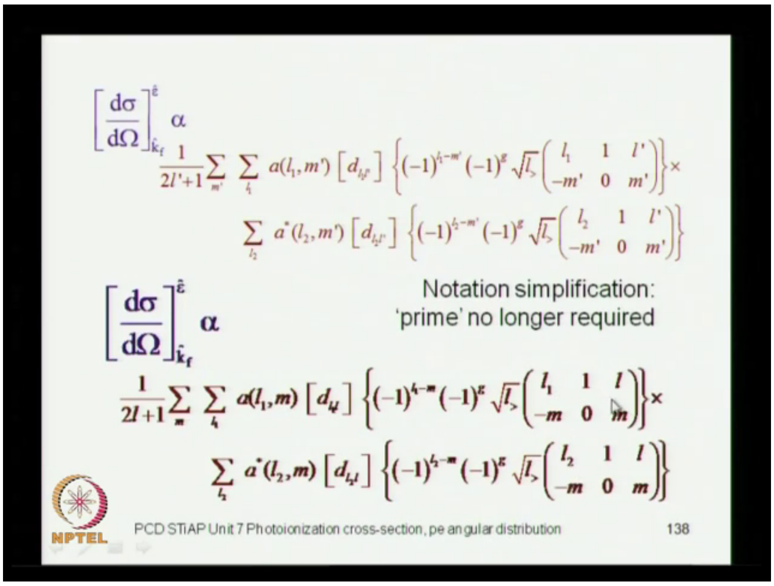

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{\varepsilon}} \alpha$$

$$\frac{1}{2l'+1}\sum_{m'}\sum_{l_1} a(l_1,m')\left[d_{l_1l'}\right]\left\{(-1)^{l_1-m'}(-1)^{g}\sqrt{l_>}\begin{pmatrix} l_1 & 1 & l' \\ -m' & 0 & m' \end{pmatrix}\right\}\times$$

$$\sum_{l_2} a^*(l_2,m')\left[d_{l_2l'}\right]\left\{(-1)^{l_2-m'}(-1)^{g}\sqrt{l_>}\begin{pmatrix} l_2 & 1 & l' \\ -m' & 0 & m' \end{pmatrix}\right\}$$

Notation simplification:
'prime' no longer required

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{\varepsilon}} \alpha$$

$$\frac{1}{2l+1}\sum_{m}\sum_{l_1} a(l_1,m)\left[d_{l_1l}\right]\left\{(-1)^{l_1-m}(-1)^{g}\sqrt{l_>}\begin{pmatrix} l_1 & 1 & l \\ -m & 0 & m \end{pmatrix}\right\}\times$$

$$\sum_{l_2} a^*(l_2,m)\left[d_{l_2l}\right]\left\{(-1)^{l_2-m}(-1)^{g}\sqrt{l_>}\begin{pmatrix} l_2 & 1 & l \\ -m & 0 & m \end{pmatrix}\right\}$$

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So, you have got plenty of summations, but you do not really need the prime anymore, because there is nothing, which we are no longer using l, because you are using l 1 and l 2, so you do not need the prime any more. So, I drop the prime in this relation now, if the same relation written with l instead of l prime, just to make the notation a little simpler, we do not need the prime any more. We needed it only when we were distinguishing between l and m prime, but for l, we have used l 1 and l 2, so we do not have l anymore. So, that is a reason we can do away with the prime now, so you have got l 1 here and l 2 here and l over here, instead of l prime. So, that was the orbital angular momentum quantum number we have used for the initial state.

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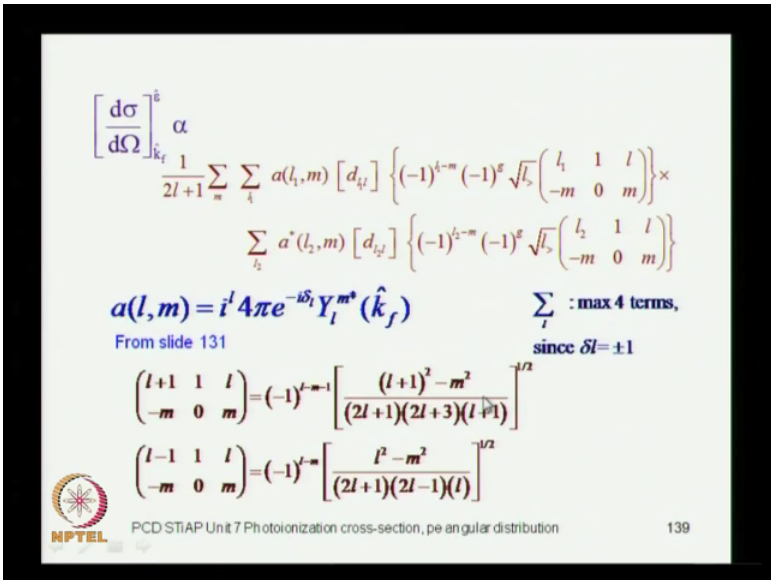

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{\varepsilon}} \alpha$$

$$\frac{1}{2l+1}\sum_m \sum_{l_1} a(l_1,m)\left[d_{l_1 l}\right]\left\{(-1)^{l_1-m}(-1)^g\sqrt{l_>}\begin{pmatrix} l_1 & 1 & l \\ -m & 0 & m \end{pmatrix}\right\}\times$$

$$\sum_{l_2} a^*(l_2,m)\left[d_{l_2 l}\right]\left\{(-1)^{l_2-m}(-1)^g\sqrt{l_>}\begin{pmatrix} l_2 & 1 & l \\ -m & 0 & m \end{pmatrix}\right\}$$

$$a(l,m) = i^l 4\pi e^{-i\delta_l} Y_l^{m*}(\hat{k}_f)$$

From slide 131

$\sum_l$: max 4 terms,

since $\delta l = \pm 1$

$$\begin{pmatrix} l+1 & 1 & l \\ -m & 0 & m \end{pmatrix} = (-1)^{l-m-1}\left[\frac{(l+1)^2 - m^2}{(2l+1)(2l+3)(l+1)}\right]^{1/2}$$

$$\begin{pmatrix} l-1 & 1 & l \\ -m & 0 & m \end{pmatrix} = (-1)^{l-m}\left[\frac{l^2 - m^2}{(2l+1)(2l-1)(l)}\right]^{1/2}$$

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So, this is what we have got and now, a l m’s, we already have from our earlier discussion. And because we are using the dipole approximation, you do not have to worry about summation over l 1 and l 2 going from 0 through infinity. Because, only those transitions will take place, for which delta l is equal to either plus 1 or minus 1, everything else will vanish, that these selection rules again as we have discussed earlier come from the Wigner Eckart theorem.

So, delta l is equal to plus 1 or minus 1 and it is because we have the dipole approximation, which is the operator which comes in when you set e to the i k dot r equal to 1 by ignoring higher powers of r over lambda. So, it is a low energy approximation and in this approximation, you have only delta l equal to plus or minus 1. And from these double summations, you can have a maximum of four terms, two terms coming from one corresponding to delta l equal to plus or minus 1 and another two coming from the other summation over l 2.

So, at the most you have to work with four terms so that, really makes life easy, all of these infinite summations immediately collapse into, just no more than four terms, so that should make us happy. And then all we have to do, is to get the values of the Wigner 3 j and these are available in various stables of angle of momentum coefficient in Schiff's quantum mechanics or Lanthanium Schiff's or any book, an angular momentum algebra will give you standard tables, you can also get them from first principles using the recursion relations, so that is not a big deal. So, you evaluate these, which are given by the factors, which I have written over here, so these are the values of the 3 j's.

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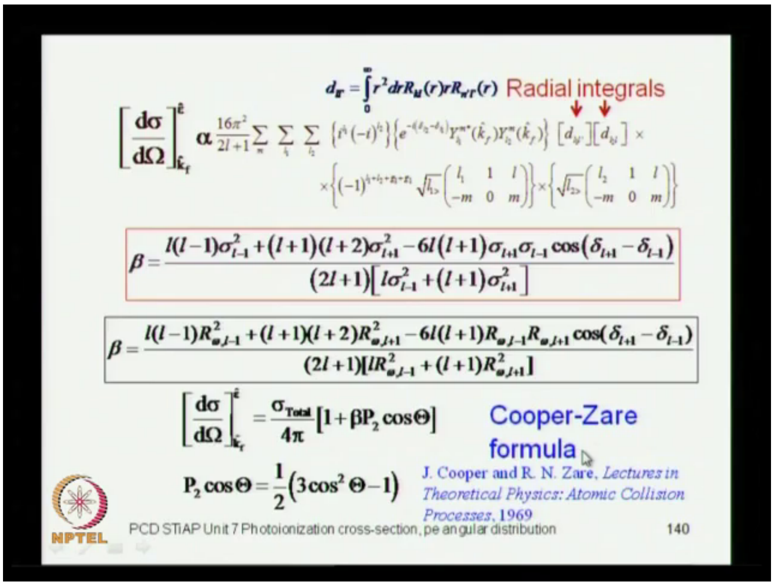

$$d_{ll'} = \int_0^\infty r^2 dr R_{nl}(r) r R_{\kappa l'}(r)$$ Radial integrals

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{\varepsilon}} \alpha \frac{16\pi^2}{2l+1}\sum_m \sum_{l_1} \sum_{l_2} \left\{i^{l_1}(-i)^{l_2}\right\}\left\{e^{-i(\delta_{l_2}-\delta_{l_1})}Y_{l_1}^{m*}(\hat{k}_f)Y_{l_2}^{m}(\hat{k}_f)\right\}\left[d_{l_1 l}\right]\left[d_{l_2 l}\right]\times$$
$$\times\left\{(-1)^{l_1+l_2+m+m}\sqrt{l_{1>}}\begin{pmatrix} l_1 & 1 & l \\ -m & 0 & m \end{pmatrix}\right\}\times\left\{\sqrt{l_{2>}}\begin{pmatrix} l_2 & 1 & l \\ -m & 0 & m \end{pmatrix}\right\}$$

$$\boxed{\beta = \frac{l(l-1)\sigma_{l-1}^2 + (l+1)(l+2)\sigma_{l+1}^2 - 6l(l+1)\sigma_{l+1}\sigma_{l-1}\cos(\delta_{l+1}-\delta_{l-1})}{(2l+1)\left[l\sigma_{l-1}^2 + (l+1)\sigma_{l+1}^2\right]}}$$

$$\boxed{\beta = \frac{l(l-1)R_{\omega,l-1}^2 + (l+1)(l+2)R_{\omega,l+1}^2 - 6l(l+1)R_{\omega,l-1}R_{\omega,l+1}\cos(\delta_{l+1}-\delta_{l-1})}{(2l+1)[lR_{\omega,l-1}^2 + (l+1)R_{\omega,l+1}^2]}}$$

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{\varepsilon}} = \frac{\sigma_{Total}}{4\pi}\left[1+\beta P_2 \cos\Theta\right]$$

Cooper-Zare formula

$$P_2 \cos\Theta = \frac{1}{2}\left(3\cos^2\Theta - 1\right)$$

J. Cooper and R. N. Zare, *Lectures in Theoretical Physics: Atomic Collision Processes*, 1969

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So, now, you have got everything, except for the radial integrals and the a l m's, which include the spherical harmonics, the phase shift and so on. The phase shifts are e to the i delta terms, so these include the cosine delta and the sin delta terms, so these are the trigonometric functions, the cosine delta and the sin delta term. So now, you can write this whole expression in terms of trigonometric functions and the radial integrals, which and there are two of them, so you have will get an expression, which is quadratic in the radial integrals.

What else will it include, it will include the phase shifts and the phase shifts will appear as arguments of trigonometric functions as cosine and sin term. So, what COOPER ZARE did was, to introduce a parameter which includes these terms, so there is a quadratic term in the radial integral, which is sigma. So, sigma l minus 1 is the radial integral from l prime to l prime minus 1, so that is the transition to the final state in the continuum, whose orbital angular momentum quantum numbers is less by 1 compared to that of the initial state.

So, there is a term in sigma l minus 1 square, there is a term in sigma l plus 1 square and there is a cross term in sigma l plus 1 and sigma l minus 1. Then there are the phase shifts, they appeared over here, they come as a difference of this cosine argument. So, this is manipulating that trigonometric terms, so it is a little bit of algebra that one has to do and COOPER ZARE were able to put it in a form, which is extremely compact by introducing this parameter.

So, this parameter is a dynamical parameter, it is of course a function of energy, because your matrix element depend on energy, your phase shifts depend on energy, so it is an energy parameter. And by introducing this parameter, you can write this expression, which is a rather complicated expression, but you can present it in very simple of form, which is called as a COOPER ZARE formula. So, this radial integrals are in some people written as sigma, we have used d over here and in some literature, they have used capital R, now this capital R is not the radial function, it is this radial integral.

So, the notation is different in different pieces of literature, so that need not confuse you, so when you see a quadratic term over here, whether it is sigma or this capital R or this d square, you know it is a radial integral and you know that, this is the radial integral that is been referenced. So, these are various notations, which are used in literature and using this expression for beta, the differential cross section, which seems to have a rather complicated structure, can now be written in a very simple form, which is sigma over 4 pi 1 plus beta times this Lagrangian polynomial for l equal to 2.

Lagrangian polynomial for l equal to 2, is this half of 3 cos square theta minus 1 and this parameter has got the information, which you need to get the angular distribution, because we are developing the expression for the differential cross section. So, d sigma by d omega is the differential cross section, it is a measure of transition probability corresponding to photoelectron escape in a given direction. What is the direction of escape, it is along k f, it is along the unit vector k f, corresponding to electromagnetic radiation being polarized along certain direction, which we have refer to as epsilon.

In our analysis, we have taken it to be the X axis, but it can be any direction in space, it does not matter, but with a reference to that, this uppercase theta is the polar angle corresponding to that direction, whatever it is, that is what we are found. So, with reference to the direction of polarization of the electromagnetic radiation, theta is the corresponding polar angle. It is not the polar angle with respect to the Z axis of the original geometry that we have, but it is the polar angle with reference to the direction of polarization of the electromagnetic radiation.

So, this is the theta and this is the measure of, how much of photoelectron yield you will expect in this direction for this direction of polarization, it is a measure of that. And it is given by this total cross section, it is a certain part of the total cross section, because when you integrate this overall angles, you will get the total cross section. So, you need to integrate this over all the angles to get the total cross section, but this is a part of the total and this part is the corresponding part, which is relevant to the direction theta.

So, if you keep a detector in the direction theta, this is what you are going to measure, this is the amount of yield that you will measure with reference to certain collaboration procedure. So, essentially, beta is then giving you the angular distribution, which is why it is called as a photoelectron angular distribution parameter. This is again in the dipole approximation, so this is called as the dipole angular distribution asymmetry parameter. So, this is the COOPER ZARE formula and I have uploaded the COOPER ZARE paper at our course web page, so you can go through the details in this paper.

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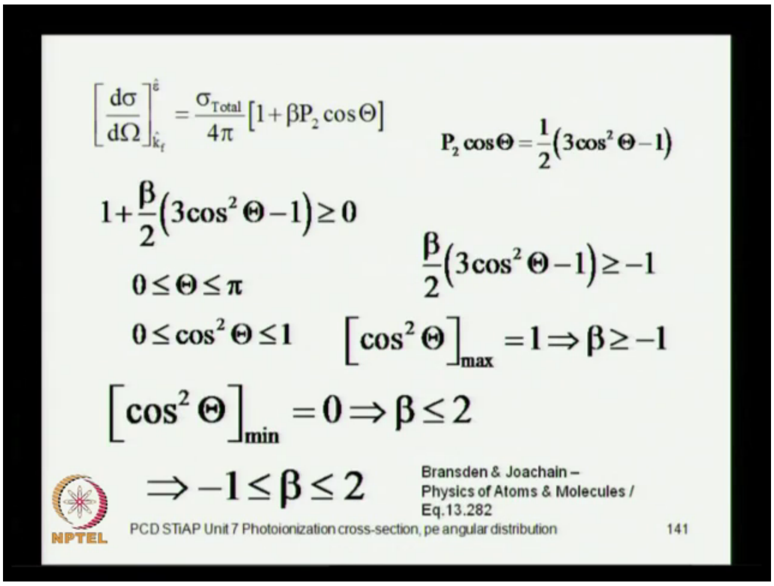

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{\varepsilon}} = \frac{\sigma_{Total}}{4\pi}\left[1+\beta P_2\cos\Theta\right]$$

$$P_2\cos\Theta = \frac{1}{2}\left(3\cos^2\Theta-1\right)$$

$$1+\frac{\beta}{2}\left(3\cos^2\Theta-1\right)\ge 0$$

$$\frac{\beta}{2}\left(3\cos^2\Theta-1\right)\ge -1$$

$$0\le\Theta\le\pi$$

$$0\le\cos^2\Theta\le 1 \qquad \left[\cos^2\Theta\right]_{max} = 1 \Rightarrow \beta\ge -1$$

$$\left[\cos^2\Theta\right]_{min} = 0 \Rightarrow \beta\le 2$$

$$\Rightarrow -1\le\beta\le 2$$

Bransden & Joachain –
Physics of Atoms & Molecules /
Eq.13.282

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And this is now, a summary of what we have got, this is the differential cross section, which is now written in very compact form, which is part of sigma, sigma divided by 4 pi and then you have got the 1 plus beta and the Lagrangian polynomial for l equal to 2. So, beta is angular distribution asymmetry parameter, now differential cross section of course, is a positive quantity, it is transition probability. So, it is a positive quantity, it has to be greater than or equal to 0.

Therefore, 1 plus beta times P 2 cos theta must be greater than or equal to 0 and that put some limits on beta, that automatically generates some limits on beta. What are those limits, because this beta over 2 times this, must be greater than or equal to minus 1 and theta can only take values between 0 and pi, corresponding to which cos square theta can take values only between 0 and 1. So, those are the minimum and the maximum values of cos square theta.

So, if you put the corresponding values minimum and maximum values of cos square theta over here, you will get the minimum and maximum value that beta can take. So, what are those, so if you take cos square theta, the maximum value is 1, so beta has to be greater than or equal to minus 1 and cos square theta minimum value is 0, so beta has to be less than or equal to 2. So, these are l m s of angular distribution asymmetry parameter, it can at the least be minus 1 and at the most it can be plus 2. So, you will always find angular distribution asymmetry parameter in these limits and you can find the discussion of this also in Bransden and Joachain book or in Fano and Cooper and the Fano and Rau and the number of other sources.

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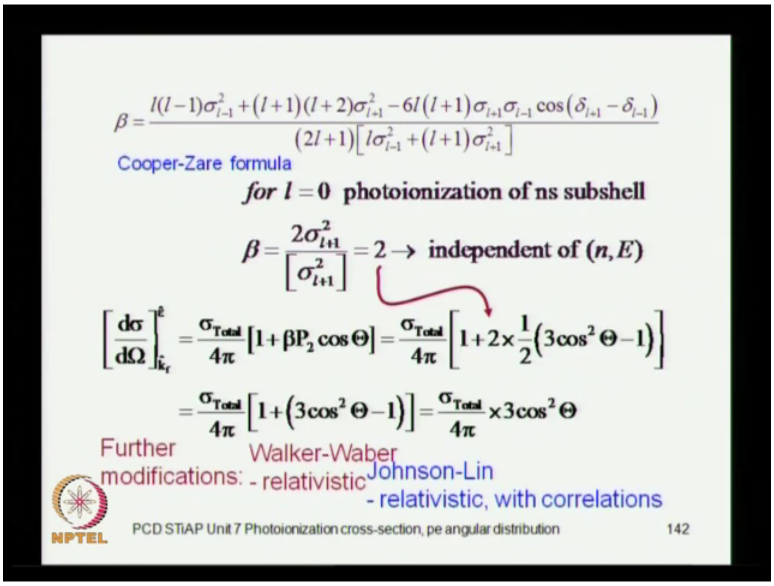

$$\beta = \frac{l(l-1)\sigma_{l-1}^2 + (l+1)(l+2)\sigma_{l+1}^2 - 6l(l+1)\sigma_{l+1}\sigma_{l-1}\cos(\delta_{l+1}-\delta_{l-1})}{(2l+1)\left[l\sigma_{l-1}^2 + (l+1)\sigma_{l+1}^2\right]}$$

Cooper-Zare formula

for $l = 0$ **photoionization of ns subshell**

$$\beta = \frac{2\sigma_{l+1}^2}{\left[\sigma_{l+1}^2\right]} = 2 \rightarrow \textbf{independent of } (n, E)$$

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{\epsilon}} = \frac{\sigma_{Total}}{4\pi}\left[1+\beta P_2 \cos\Theta\right] = \frac{\sigma_{Total}}{4\pi}\left[1+2\times\frac{1}{2}\left(3\cos^2\Theta-1\right)\right]$$

$$= \frac{\sigma_{Total}}{4\pi}\left[1+\left(3\cos^2\Theta-1\right)\right] = \frac{\sigma_{Total}}{4\pi}\times 3\cos^2\Theta$$

Further modifications: Walker-Waber - relativistic

Johnson-Lin - relativistic, with correlations

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So, this is the COOPER ZARE formula for the angular distribution of photoelectrons, now let us take a special case, if you study photoionization of l equal to 0 and it does not matter what the m quantum number is. Because, for l equal to 0, this term will vanish, this is l into l minus 1, this term is 6 into l time something, so this will also vanish. This is l plus 1 times l plus 2, so l is equal to 0, so this is 1 and this is 2, so you get twice sigma square in the numerator and in the denominator l equal to 0.

So, 2 l will be 0 and this will be one time at rest, again l is 0 via, so this term is vanish and you will have the remaining term, which is l plus 1, which is 0 plus 1, so it is again sigma square. So, you get 2 sigma square over sigma square, corresponding to the transition dealt l is equal to plus 1. And the radial integral contribution, the quadratic term in the radial integral in the numerator and the denominator cancel each other, it does not matter what the value is.

So, no matter what energy you are talking about, the radial integral is a function of energy of course, the phase shifts are functions of energy, it does not matter, whatever they are, beta turns out to be a constant number which is equal to 2. So, for photoionization from the n s sub shell, it does not matter what is the value of n, 1 s 2 s 3 s 4 s whatever. For photoionization from the n s sub shell of any atom, beta must always be equal to 2 and independent of the principle quantum number, also independent of n E.

And you can develop similar relations for other values of l, for special cases for example, we have discussed Cooper minimum and when you have the Cooper minimum in the l plus 1 channel for example. If the transition corresponding to delta l equal to plus 1, that matrix element is going through 0, which is a Cooper minimum then sigma l plus 1 will go to 0 over there. This sigma l plus 1 will also go to 0 and then you will have only the remaining terms.

So, you can simplify the expressions for beta for special cases, where you have Cooper minimum, either in the l plus 1 channel or even in the l minus 1 channel. But, typically you have Cooper minimum in the l plus 1 channel, but that is a matter of detail that you can read in Fano and Cooper's paper. So now, for s sub shell, if you look at the expression for the differential cross section for the special case of l equal to 0, which is a photoionization of the n s sub shell, when you put beta equal to 2 in this expression over here and you get this simple cos square theta distribution.

So, photoionization from all s sub shells will be typically given by this cos square dependence. Now, there are of course further modifications, because we have used a non relativistic approximation. So, when you do this whole analysis using relativistic consideration, you will have transitions, two different final states, which are split by the spin orbit interaction. And there will be a spin orbit splitting also in the initial state, so there are some details that you need to consider.

And then the relativistic formula which we will not discuss is, what is given by Walker and Waber and then we have still not taken into account, even after taking into account relativistic interactions, you have to plug in other details, because there of course, are the electron correlations in many electron atoms that you must include. So, you have to include relativistic corrections, you also have to introduce many body corrections due to the coulomb correlation.

And these are not included in the Hartree Fock or even in the direct Hartree Fock, which is the relativistic self consistent field study. Even then in the relativistic self consistent field, you do not have the electron correlation and you must take those into account. And this is a matter of details, which goes beyond the scope of our discussion in this course. But then they have been studies, in which these correlation have been included and the relativistic many body correlations. Those expressions are developed by Johnson and Lin in the random phase approximation, so some of these things are matches of details for further study.

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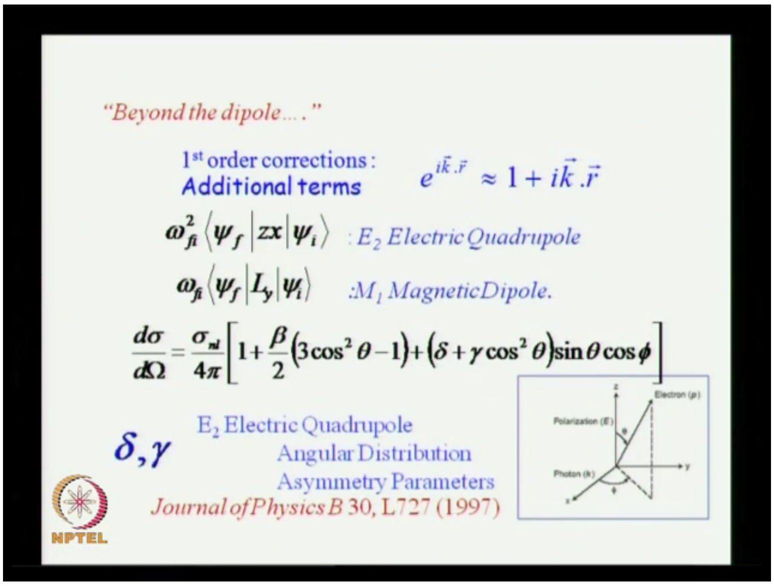

"Beyond the dipole…."

1st order corrections:
Additional terms $e^{i\vec{k}.\vec{r}} \approx 1 + i\vec{k}.\vec{r}$

$\omega_{fi}^2 \langle \psi_f | zx | \psi_i \rangle$: E_2 Electric Quadrupole

$\omega_{fi} \langle \psi_f | L_y | \psi_i \rangle$: M_1 Magnetic Dipole.

$$\frac{d\sigma}{d\Omega} = \frac{\sigma_{nl}}{4\pi}\left[1 + \frac{\beta}{2}(3\cos^2\theta - 1) + (\delta + \gamma\cos^2\theta)\sin\theta\cos\phi\right]$$

δ, γ E_2 Electric Quadrupole
Angular Distribution
Asymmetry Parameters
Journal of Physics B 30, L727 (1997)

And then of course, one can also go beyond the dipole, because the dipole approximation essentially by it is very name as we know it, is an approximation. Because, we have truncated e to the i k dot r only equal to 1, is what gives us the dipole approximation. If you take the next term, you already go beyond the dipole and this will already introduce certain corrections. So, what kind of corrections as it introduce, you need to consider matrix elements of some other operators.

It is not just a dipole operator, but you get the some other operators like the electric quadruple operator and the magnetic dipole operator. So, these get into the picture and you have to include corrections for these when you go beyond the dipole approximation and what was left out of the COOPER ZARE formula. The COOPER ZARE formula had only this dipole angular distribution, it had only this beta over 2 times 3 cos square theta minus 1.

But now, you have additional terms and delta and gamma are now the non dipole angular distribution asymmetry parameters. So, you have to go beyond the dipole approximation, as a matter of fact, even at low energies means, we have argued that, the dipole approximation is a good approximation for low energies, it is a high wavelength approximation. But then nevertheless it is an approximation and then even at low energy, sometimes depending on the kind of measurement you are carrying out and you can carry out extremely high precision measurements.

Because, now the electronics is very powerful, the detection devices are very powerful, light sources are very powerful. Typically these measurements are done at synchrotron radiation laborites, where we have got a very powerful light source over a wide spectrum of energies, over large wave length regions. And in India, these experiment are now possible at the Indus synchrotron and that is only place, where we have synchrotron in India.

But, there are good number of synchrotron in the world and many of these measurements are carried out at various synchrotron laboratories. And you can actually measure these non dipole angular distribution asymmetric parameters and the theory has to be good enough to be able to correspond to those experiments. So, it has to include relativistic effect, it also has to include the many body correlation effects. So, these are the non dipole angular distribution asymmetry parameters delta and gamma and here is the reference, in which you can read further about it.

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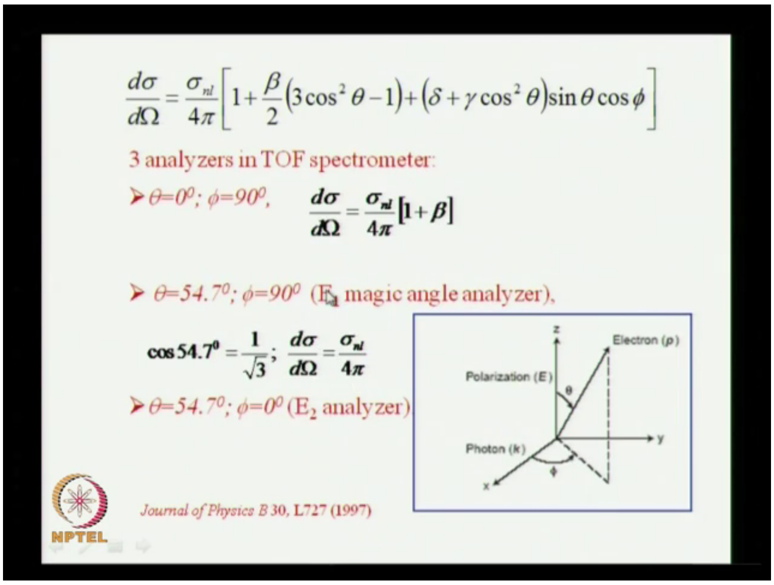

$$\frac{d\sigma}{d\Omega} = \frac{\sigma_{nl}}{4\pi}\left[1 + \frac{\beta}{2}\left(3\cos^2\theta - 1\right) + \left(\delta + \gamma\cos^2\theta\right)\sin\theta\cos\phi\right]$$

3 analyzers in TOF spectrometer:

- $\theta=0^0$; $\phi=90^0$, $\frac{d\sigma}{d\Omega} = \frac{\sigma_{nl}}{4\pi}[1+\beta]$
- $\theta=54.7^0$; $\phi=90^0$ (E_1 magic angle analyzer),

$$\cos 54.7^0 = \frac{1}{\sqrt{3}};\ \frac{d\sigma}{d\Omega} = \frac{\sigma_{nl}}{4\pi}$$

- $\theta=54.7^0$; $\phi=0^0$ (E_2 analyzer)

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So, one can carry out measurements, which are really very interesting, there is a may technique which is known as the time of flight spectrometer. And you can setup three time of flight spectrometers and finally, these are measurements which experimentally carry out. And you locate these detectors not over all space, because you do have to get angular distributions, it does not mean that, you have to carry out measurements at every single angle.

You can get all that information by carrying out measurements only at some of the angle and then get information about everything else. So, how do you do that, in fact if you have 3 analyses in the time of flight spectrometer, one at theta equal to 0 and pi equal to 90 degrees, another at 54.7 degree and phi equal to 90 degrees and another at 54.7 degree theta and phi equal to 0 degrees. Then you can get all of these information how, because what happens at theta equal to 0, sin theta vanishes, so the these terms go away.

And at 54.7, the cosine term gives you 1 over root 3 cosine of 54.7 is 1 over root 3, so you got the square of that, so that one third, so one third times 3 will give you 1, so 1 minus 1 vanishes. And pi is 90, so cosine pi is 0 and what you get, you get d sigma by d omega equal to the total cross section divided by 4 pi. So, by just carrying out measurement at just this one angle, just one angle single angle, you get a total cross section.

So, it is like magic, which why it is magic angle.

Student: ((Refer Time: 45:17))

Because, it depends on n and l quantum numbers, it is for a particular n l initial state, all the terms are l dependent.

Student: ((Refer Time: 45:38))

Yes, the expression for beta, the angular distribution asymmetry parameter, it has got l everywhere.

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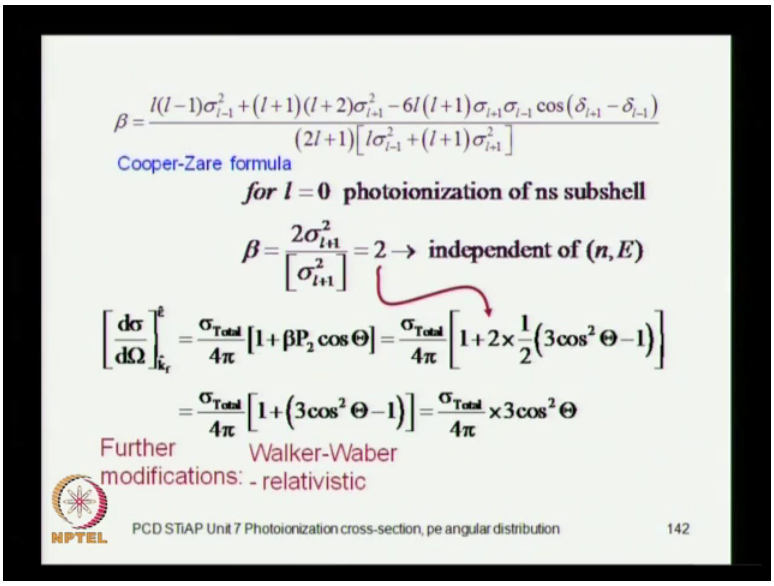

$$\beta = \frac{l(l-1)\sigma_{l-1}^2 + (l+1)(l+2)\sigma_{l+1}^2 - 6l(l+1)\sigma_{l+1}\sigma_{l-1}\cos(\delta_{l+1}-\delta_{l-1})}{(2l+1)\left[l\sigma_{l-1}^2 + (l+1)\sigma_{l+1}^2\right]}$$

Cooper-Zare formula

for $l = 0$ **photoionization of ns subshell**

$$\beta = \frac{2\sigma_{l+1}^2}{\left[\sigma_{l+1}^2\right]} = 2 \rightarrow \text{independent of } (n, E)$$

$$\left[\frac{d\sigma}{d\Omega}\right]_{\hat{k}_f}^{\hat{e}} = \frac{\sigma_{Total}}{4\pi}\left[1+\beta P_2 \cos\Theta\right] = \frac{\sigma_{Total}}{4\pi}\left[1+2\times\frac{1}{2}\left(3\cos^2\Theta-1\right)\right]$$

$$= \frac{\sigma_{Total}}{4\pi}\left[1+\left(3\cos^2\Theta-1\right)\right] = \frac{\sigma_{Total}}{4\pi}\times 3\cos^2\Theta$$

Further modifications: Walker-Waber - relativistic

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Look at this, so this certainly depends on the orbital angular quantum number of the initial state, but this is the non relativistic expression. In the relativistic expression, you need the Kappa quantum number, not the l. So, beta of course, is l dependent, so the differential cross section is for a given initial state, which is describe by n and l in non relativistic quantum mechanics, which is the expression that we have. But then in the relativistic expression, you will have the Kappa quantum number, which we have discussed, rather than the l quantum number.

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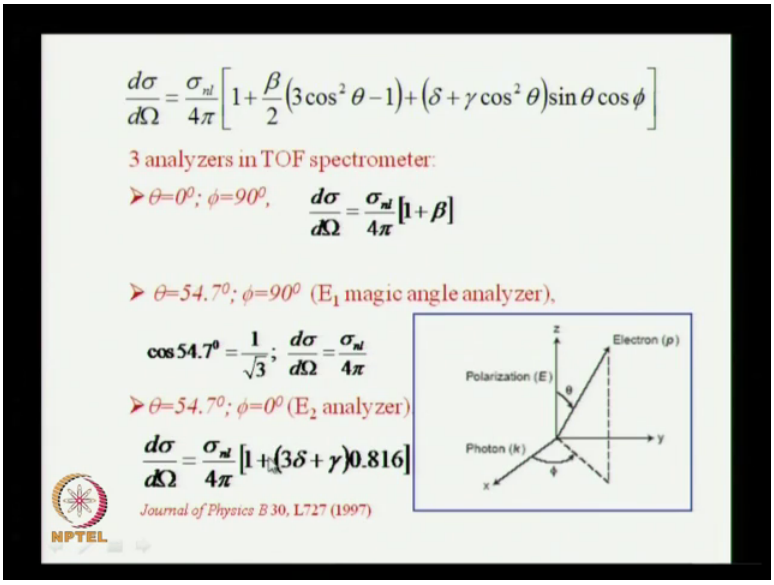

$$\frac{d\sigma}{d\Omega} = \frac{\sigma_{nl}}{4\pi}\left[1 + \frac{\beta}{2}\left(3\cos^2\theta - 1\right) + \left(\delta + \gamma\cos^2\theta\right)\sin\theta\cos\phi\right]$$

3 analyzers in TOF spectrometer:

- $\theta = 0^0$; $\phi = 90^0$, $\frac{d\sigma}{d\Omega} = \frac{\sigma_{nl}}{4\pi}[1+\beta]$
- $\theta = 54.7^0$; $\phi = 90^0$ (E_1 magic angle analyzer),

$\cos 54.7^0 = \frac{1}{\sqrt{3}}$; $\frac{d\sigma}{d\Omega} = \frac{\sigma_{nl}}{4\pi}$

- $\theta = 54.7^0$; $\phi = 0^0$ (E_2 analyzer)

$$\frac{d\sigma}{d\Omega} = \frac{\sigma_{nl}}{4\pi}\left[1 + (3\delta + \gamma)0.816\right]$$

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And you have at this magic angle, you can get the total cross section by carrying out measurement just at this angle, which is called as a magic angle. Then you can carry out measurement at pi equal to 0 and at phi equal to 0, cosine phi will be 1 and then sin theta which is sin of 54.7 is 0.816. But then this is the magic angle, so this term will vanish and the dipole terms go away and you get only the non dipole angular distribution parameters from this.

So, sometimes this is very important analyzer, because you get the non dipole parameters from this. So, if by carrying out these measurements intelligently by setting up your detectors at very special angles, you can get a lot of information. So, you can get some references over here in this paper.

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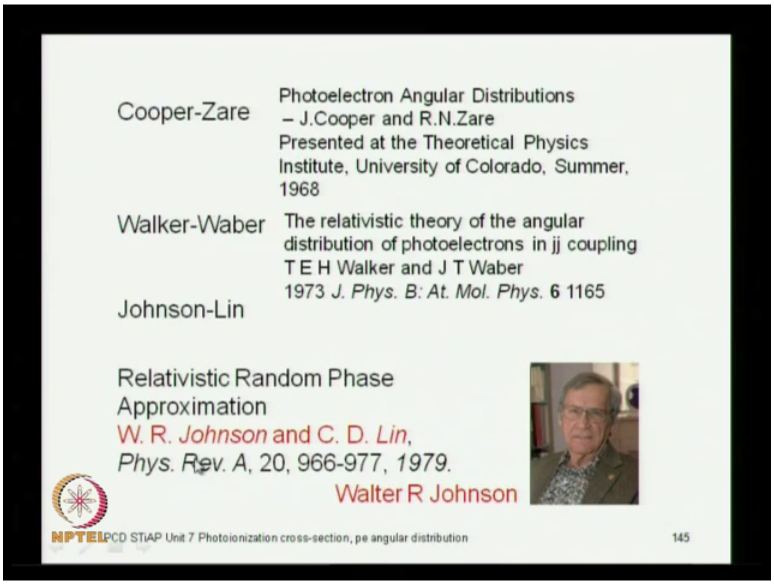

Cooper-Zare

Photoelectron Angular Distributions
– J.Cooper and R.N.Zare
Presented at the Theoretical Physics Institute, University of Colorado, Summer, 1968

Walker-Waber

The relativistic theory of the angular distribution of photoelectrons in jj coupling
T E H Walker and J T Waber
1973 *J. Phys. B: At. Mol. Phys.* **6** 1165

Johnson-Lin

Relativistic Random Phase Approximation
W. R. *Johnson* and C. D. *Lin*,
Phys. Rev. A, 20, 966-977, *1979.*

Walter R Johnson

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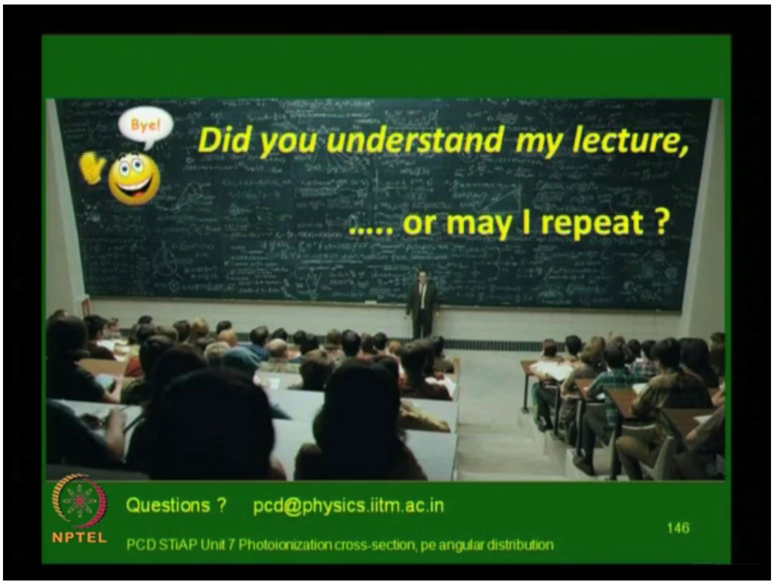
So, I will give you some of the essential references then we conclude discussion on the angular distribution of photoelectrons and also this unit. So, this is the classic paper by COOPER ZARE, which I have uploaded on our course webpage already, the Walker Waber gives you the relativistic formula. And then when you include the electron correlations, then of course, you do not have exact solutions, when you have a many body problem, you do not have exact solutions.

So, one of the very powerful method to include the electron correlation, even if it not exact and there is no exact solution, but one of the very powerful techniques is, what is called is a relativistic random phrase approximation developed by Johnson and Lin. And you will find the expression for the angular distribution asymmetry parameters developed in this paper by Johnson and Lin and with that, I will conclude. But then my usual goodbye slide, I thought I will modify a little bit, because I found one interesting slide on the internet, which will ensure that, you have understood everything that I have said.

(Refer Slide Time: 48:40)



Did you understand my lecture,

….. or may I repeat ?

Questions ? pcd@physics.iitm.ac.in

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It will give you some confidence in what you have learnt, because I am sure you are going to say yes, you do not want to continue the class. So, by saying yes, you will gain some confidence, so thank you very much. If there any questions, if you are really not understand something, please ask, I am very happy to answer, but otherwise say yes and go with confidence that you have understood everything or also I repeat, questions.

Student: ((Refer Time: 49:17))

In the non relativistic approximation, this is the non relativistic, relativistically you have transitions to the singular ((Refer Time: 49:27)). And you can have the matrix element changing and beta can actually go to minus 1 at Cooper minimum in one of the two chance, even for us, even for low Z atoms. So, sometimes you have relativistic effects become extremely important means, the usual belief is, that they are important only for high Z atoms, but even for low Z atoms.

Because, you have these two channels and the Cooper minimum in one channel, beta can go to minus 1, it can also go to minus 1 in the region of photoionization resonances. So, these are the several details that one can discuss and go beyond this. But, I hope that, this will introduce you to original literature in this field, any other question.

Thank you very much.