

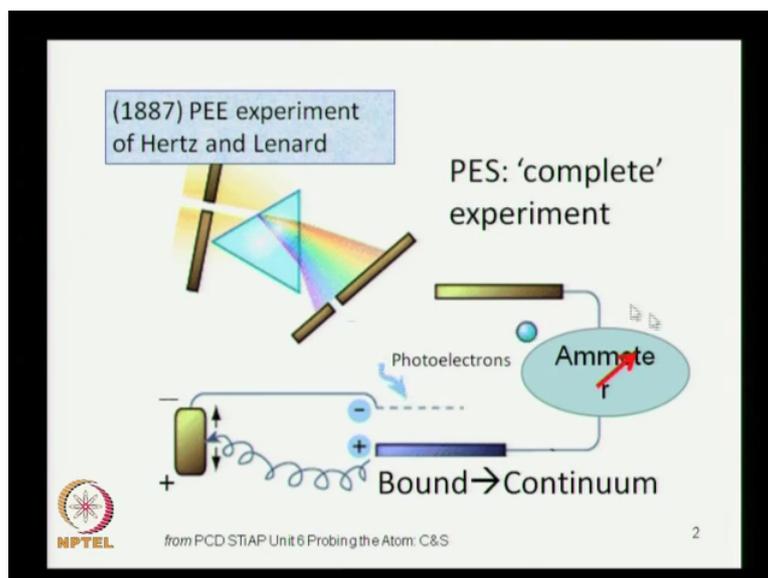
**Select/Special Topics in Atomic physics**  
**Prof. P.C. Deshmukh**  
**Department of Physics**  
**Indian Institute of Technology, Madras**

**Lecture - 30**

**Atomic Photoionization Cross-Sections, Angular Distribution of Photoelectrons**

Greetings, we begin a new unit today, the 7th unit of this course on Atomic Photoionization. And we will begin to see the applications of the quantum kinetics that we have developed in earlier units and they will all come together, when we get into these applications. And I will introduce you to photo ionization cross sections angular distributions of photo electrons and some of the other properties.

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So, this is the experiment that really contributed a lot to quantum kinetics, because it was the interpretation of this which really led to the understanding of the quantization of the electromagnetic field. And so this was a fantastic experiment done by Hertz and Leonard and its explanation in 1905 by Einstein is what led to the formulation of quantum kinetics.

So, you have these photo electrons coming out from this metal plate when light falls on it. And in high school when you study about this experiment and about quantization of energy, you only look at the energy consideration that there is a conservation of energy and the kinetic energy of the photo electrons is just a statement of conservation of energy from the photon energy you remove the binding energy you get the kinetic energy right. But, there

is so much more to this experiment, because a physicist likes to do a complete experiment as get maximum information about the system, which is being investigated.

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The slide features three portraits: Hertz (1887), Lenard, and Einstein (1905). To the right of the portraits is a diagram of an atom with several energy levels. A blue wavy arrow representing a photon points upwards from a lower level to a higher level. Below the portraits, the matrix element  $\langle \psi_f | T | \psi_i \rangle$  is shown with red arrows pointing to it from the portraits. Below this, a partial formula is given:  $|\psi_f\rangle \rightarrow e^{ikr} - \frac{e^{-ikr}}{r} \sum_l (2l+1) P_l(-\cos\theta) \left( \frac{e^{-i2\delta_l} - 1}{2ik} \right)$ . The NPTEL logo is in the bottom left, and the text 'from STIAP Unit 6 Probing the Atom: C&S' is at the bottom center. A small number '3' is in the bottom right corner.

So, I will talk about the complete experiment and how it is interpreted in the a context or quantum mechanics. And you have this transition from a bound state when a photon is absorbed the electron goes into the continuum. And this transition is affected, because of a certain interaction between the electromagnetic field and the quantum atomic system; so this matrix elements that you see over here, is what measures, but give us a measure of the probability amplitude for transition from an initial state to a final state.

The modulus square of this will give the transition probability and it will be proportional to the intensity of absorption. So, the photo absorption cross section and so on will be related to this; so number of questions come up how do you describe the initial state, is it a non relativistic initial state, is it a relativistic initial state, does it take into account correlations, does it take into account the exchange correlations, does it also take into account the coulomb correlation.

So, there are large number of questions which can be raised, on what this initial state is, and at the simplest level it can be like a hydrogenic state, but then there are very many complex levels at which this question can be ask. And to get a really good answer one has to do a fully relativistic many body formulation quantum mechanics applied to atom, but get you know

correlated wave functions for this to describe the initial state. Then you can also ask how do you describe the coupling operator which is responsible for effecting the transition.

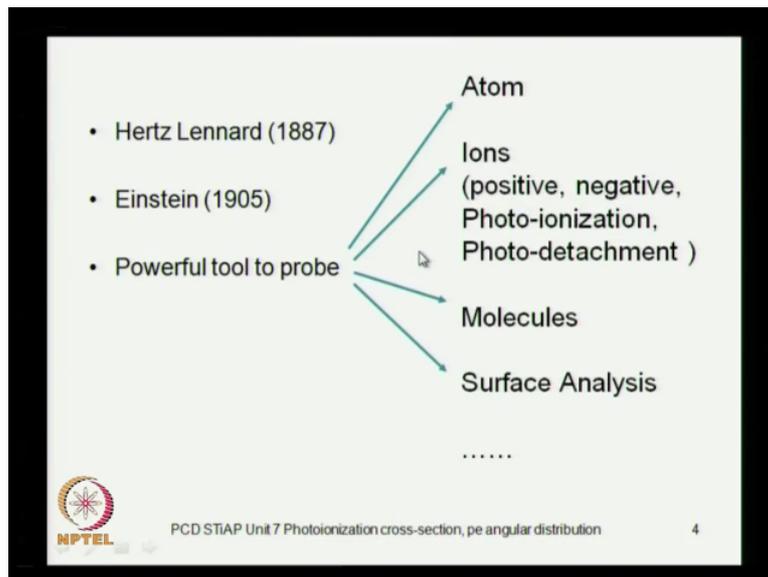
Because, there is an interaction between the electronic field and if you express the electromagnetic field as you know like  $e^{-i\mathbf{k}\cdot\mathbf{r}}$  you have got the vector potential. Then you can expand this in multiples and do you take into account all the multiples or do you take only the leading term, do you take the dipole term, do you take the quadrupole term, do you take the octupole term you know.

So, what exactly is the coupling and again you can make a number of approximations and deal with this operator  $t$ , which is responsible for effecting the transition and then the question is how does it describe the final state wave function. And here again depending on the level at which you are answering this question, you have a multiplicity of you know alternative to consider at the simplest levels this can be continuum non relativistic wave function it can be relativistic continuum functions.

Then again you can take into account the correlations and inter channel coupling in the continuum, so to get more exact answers. So, again there is a very complexity of levels and a very detailed investigation of this matrix element certainly requires a very thorough analysis of the quantum many body problem of the atomic system. Now, what we have learnt in the previous unit is that the final state wave function is a free particle solution as such and it has to be described according to the incoming wave boundary conditions.

So, at the non relativistic level we know what a wave function looks like subjected to incoming wave boundary condition and that is the solution which I have written over here; and it is precisely this form which you must use in this matrix element otherwise you will not get the right answers. If you use  $\psi_f$  without incoming wave boundary condition you will not get the correct answers for the photo ionization problem. So, that is the reason that I discussed the incoming wave boundary conditions before we came to this topic.

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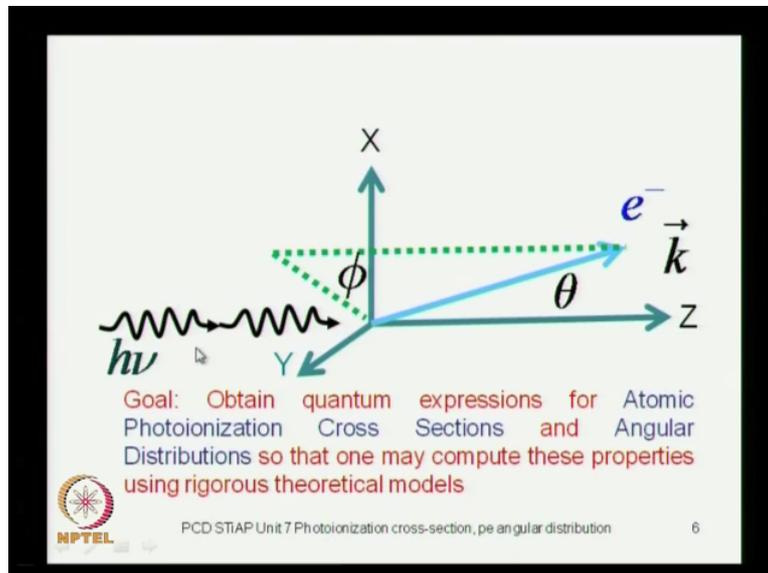
So, these are very powerful tools to study atomic systems ions also negative ions not only positive ions, when you have a negative ion you know when it absorbs energy the extra electron, which is attached in a negative ion can get detached and that process is called as photo detachment. And you would carry out similar studies on molecules as well and clusters and surfaces, so it is because a very powerful tool in surface analysis, so which is why this subject is of considerable importance and interest.

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So, you have a continuum of energies and these are the photo ionization transitions that we shall be talking about.

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So, basically if you have a coordinate system a Cartesian coordinate system and you have got incidence of electromagnetic energy along the z axis. And so you choose your z axis along the direction of incidence of the electromagnetic energy. And let us say photoelectron, the electron which is not doubt is what I shall refer to as a photo electron, so this is the photo electron which comes out it comes out in a given direction, the exit channel is unique in the photo ionization experiment as we know.

So, this is the direction let us say it goes out in the direction with a way vector  $k$  and this is the direction of ejection and with reference to the polar axis z this angle is theta; then there is a Azimuthal angle phi with respect to x axis, and we choose the x axis to be the direction of polarization of the electric intensity.

So, that will be the reference scheme and our goal is to obtain a expressions for the photo ionization cross section and the angular distribution because with the reference to the direction of incidence of the photon and with the reference to it is polarization direction what is the angle at which this electron comes out. So, that is the question which we shall take up and that is called as the angular distribution of the photoelectrons.

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- C.S.C.O.
  - Cross-sections (Probabilities)
  - Angular distribution of photoelectrons
  - Spin-polarization parameters of the photoelectrons

$\langle \Psi_f | T | \Psi_i \rangle$  Transition Matrix Element  
 T : Coupling operators
 

- Dipole
- Quadrupole
- Other ?



PCD STAP Unit 7 Photoionization cross-section, pe angular distribution 7

So, in addition to the cross sections and the angular distributions you can also measure the spin polarization parameters of the photo electrons. So, these are like compatible measurements with each other, so the uncertainty principle will allow you to carry out these measurements and which is why a complete experiment requires you to study all of these parameters not just one of those. So, I mentioned earlier that you have the coupling operator to be either the dipole or the quadruple could be any other and that again sets a level approximation and the scheme that you are implementing.

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$\langle \Psi_f | T | \Psi_i \rangle$

Continuum function with 'in-going' wave boundary condition

Initial state

- I.P.A. Non-Relativistic
- or
- H.F. Relativistic?
- D.F. "correlations"
- M.C.H.F. / M.C.D.F.

Configuration interaction in the continuum

Mg:  $1s^2 2s^2 2p_{1/2}^2 2p_{3/2}^4 3s^2$  - Inter-channel coupling

Operator T is specific to the nature of 'coupling'

$3s \xrightarrow{e_1} \epsilon p_{3/2}, \epsilon p_{1/2}$   
 $3s \xrightarrow{e_2} \epsilon d_{5/2}, \epsilon d_{3/2}$



PCD STAP Unit 7 Photoionization cross-section, pe angular distribution 8

So, you can do the initial state as I mentioned at the independent particle approximation, at the Hartree-Fock level, if you do a relativistic self-consistent field you have the direct one-particle wave functions to describe the initial state. If you take into account the electron correlations for which you will need a Multi-Configurational Hartree-Fock (MCHF), or a relativistic self-consistent field, but to take into account the correlations, which you have ignored in the Hartree-Fock at the direct one-particle level which we discussed in the earlier unit. Say, if you want to include those you will have the multi-configurational Hartree-Fock or multi-configuration direct one-particle, so that is the MCDHF. And you can describe the initial state at a variety of your known approximations or a variety of accuracies that you can go for. And then you can also take into account the configuration interactions in the continuum, so that will give you the correlations in the final state as well.

So, let me give you an example of a yawl let us take an atomic system, like the magnesium atom it is atomic number is 12 and there are this is the electron configuration at the ground state in the usual ground state of magnesium. And if you just consider the photo ionization of the outer most 3s electron, then relativistically this outer electron can go to a continuum p<sub>3/2</sub> orbital, and also to a p<sub>1/2</sub> orbital.

So, there are two possibilities, and this is again like a Young's double slit experiment that there are two possibilities and you will then therefore, expect to see some interference effects. So, when you take into account these interference effects you say that you have taken into account the configuration interactions between these two possibilities there are these two configurations one leading to a p<sub>1/2</sub> continuum state the other leading to a p<sub>3/2</sub> continuum state.

And you can take into account, the interference between this is the inter-channel coupling between these two channels. This transition is effected by  $e_1$  which is the symbol for the dipole transition and I have mentioned the dipole transition earlier. So, the dipole transitions have the selection rules  $\Delta l = \pm 1$ , so you have got a transition from s to p which is permissible under the dipole selection rules. But, then you may have as I mentioned not just the dipole transitions you may also have the quadrupole transitions and this selection rules for the quadrupole of course are different.

So, if you have a quadrupole transition, which is represented by  $e_2$  then  $\Delta l$  can actually be 2. So, you can have a transition from s to d, so you will have 2 relativistic transitions s to d

5 half and s to d 3 half, so again depending on what is the coupling operator you are making use of you would have either the dipole calculations or the quarter pole calculations right. And the atomic system when it responds to the electromagnetic energy it is going to respond in its natural way.

So, strictly speaking you really need to include all the operators, all the coupling to get the exact picture, but you can get a fairly good description of the process by making some approximations. So, that really depends on what is the accuracy of your measurement process and you know how many details you want to go, but now very sophisticated experiments can be done very high precision electronics is available very powerful light sources are available. So, you also need very rigorous theories to explain this phenomenon, which is why you need relativistic quantum many-body theories to explain these processes.

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DISCRETE EXCITATION: Photo-excitation

Photo-ionization / Photodetachment

Final state: continuum

Cross-section :  $\sigma$   
(transition probability)

Angular distribution of the photoelectrons :  $\beta, \gamma, \zeta$

Along with measurements of Spin polarization parameters

→ 'complete' experiment

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9

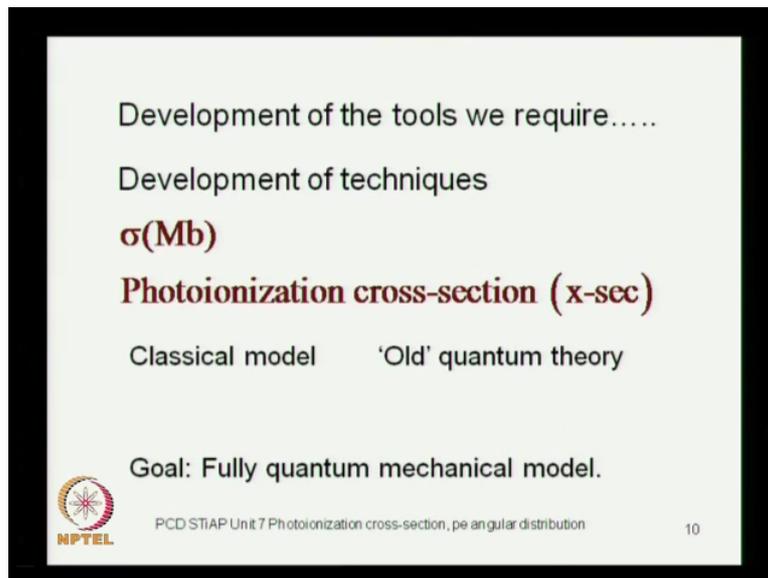
So, sometimes you have a transition just to the discrete level and that is photo excitation, but at the energy at which you have got excitation from one state, from a less bound state you could also have ionization. And then you can have interference between ionization and excitation also, so that leads to some very interesting phenomenon such as auto ionization, resonances and I will mention some of this in the later part.

So, you measure what is called as a cross section which is actually transition probability. And transition probability it is scaled according to certain relationships I will explain this and then the usual measure for the transition probability is in terms in what is called as the cross

section. You also measure for the complete measurements for the complete experiments the angular distributions of the photo electrons and this is described by a number of parameters.

So, if you have dipole approximation you have only the beta parameter, but if you also include the quarter pole parameter you have some additional parameters like gamma, beta and so on. And then along with the measurements of the spin polarization parameters you get a complete experiment and a complete description of the photo ionization process.

(Refer Slide Time: 14:13)



Development of the tools we require....

Development of techniques

$\sigma(Mb)$

**Photoionization cross-section (x-sec)**

Classical model      'Old' quantum theory

Goal: Fully quantum mechanical model.

 PCD STIAP Unit 7 Photoionization cross-section, pe angular distribution 10

So, our goal in this unit is to describe the tools, that we need to explain what photoionization cross section is, and get it is exact description. The terminology also makes use of certain classical models, because very often some of these classical ideas are used in the description of the quantum phenomenon. But, then our goal is to have a fully quantum mechanical model and it is therefore, useful to begin with the classical model and then go through these steps. So, that we do not miss out and we are we will then be well equipped to describe this process comprehensibly.

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Interaction of EM radiation with an atom

- Atomic polarizability

Oscillations of electrons about mean position.

- Polarization

Induced dipole moment

- Susceptibility

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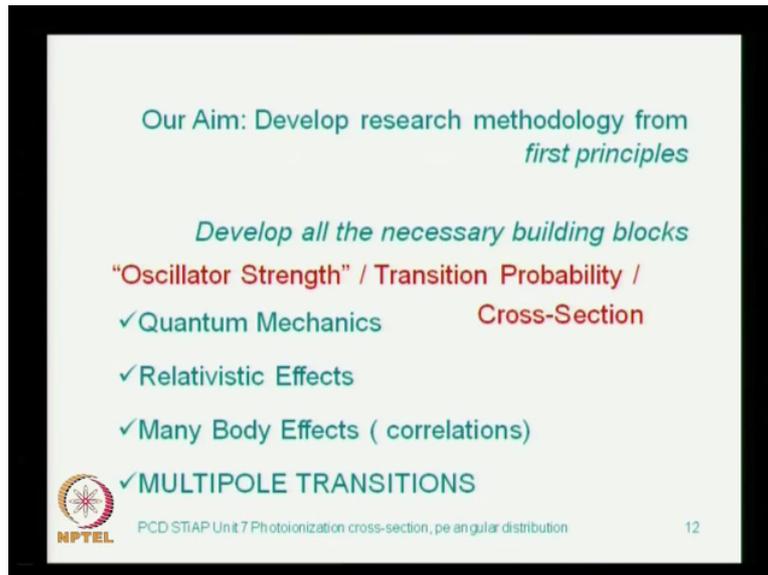
PCD STAP Unit 7 Photoionization cross-section,  $p_e$  angular distribution

11

So, essentially we are describing the interaction of a electromagnetic radiation with an atom and the classical model presumes that the electrons as it responds to the electromagnetic energy, they oscillate about a certain mean position. Now, we know that this picture is very classical and from the quantum mechanical point of view it is not correct.

But, a lot of terminology which gets carried on into quantum mechanics comes from this description, which is why I need to go through it. So, the idea here is that the electrons oscillate about a certain mean position in the atomic system and as a result of which there is an induced dipole moment, because you got a charge which is oscillating right. So, you have got an induced dipole moment, which is sets in and you will therefore, expect to meet ideas like atomic polarizability, polarization susceptibility and some of these macroscopic electromagnetic properties are then related to photo absorption cross section, so through this connection.

(Refer Slide Time: 16:02)



Our Aim: Develop research methodology from  
*first principles*

*Develop all the necessary building blocks*

**"Oscillator Strength" / Transition Probability /  
Cross-Section**

- ✓ Quantum Mechanics
- ✓ Relativistic Effects
- ✓ Many Body Effects ( correlations)
- ✓ MULTIPOLE TRANSITIONS

 PCD STAP Unit 7 Photoionization cross-section, pe angular distribution 12

So, we will develop all the necessary building blocks for this process. So, we will define what is called as oscillator strength. The term oscillator strength comes from these oscillations which I have already mentioned, so I will define it rigorously. And this will be related to the quantum mechanical transitional probability, and then to the cross section which is the common parameter in terms of which the transition probability is measured.

So, we will need all of the tools quantum mechanics relativistic effects many body effects multi pole transitions all of these will come together, but we will build the model from the round up. So, that we know where the term oscillator strength, comes from and how it connects to the quantum mechanical cross section.

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Simplest level: atomic electrons 'driven' by  
Electric Intensity Vector of EM field:

$e$  : electron's charge  $\hat{\epsilon} E_0 e^{-i(\omega t + \theta)}$

Each electron in an atom is bound to its  
site by a restoring force  $-k\vec{r}(t)$

$$m\ddot{\vec{r}}(t) = -k\vec{r}$$

U: Fano & J.W. Cooper  
Review of Modern Physics 40:3 441 (1968)



PCD STIAP Unit 7 Photoionization cross-section, pe angular distribution 13

First principles is from ground up, so we do not make too many assumptions, we state our postulates from the very beginning, so that we do not have to make too many assumptions. So, we begin with first principles and build on that in a logical way, so that we there will be no gaps in our understanding, so that is the idea.

So, you have an electromagnetic field whose electric intensity vector is described by this vector here, which is  $e_0 e^{-i\omega t}$  with a certain phase factor. Let us say the electrons charge is  $e$ , a classic reference for this is a review by Fanno and Cooper in 1968, which I have referred to I will also have it uploaded on the course web page, it is a very good paper which describes the phenomenon. And since our model is one of oscillations effected by this, you presume that the motion is described this is the classical picture which is mass times acceleration.

So, this is essential the Newton's law that we have written over here and there is a restoring force. So, there is a certain restoring spring constant which is  $k$ , and this is the simple harmonic oscillator of our model where in the oscillations are set in by the electromagnetic field.

(Refer Slide Time: 18:31)

**Damped oscillator**

$$m \ddot{\vec{r}}(t) = -k \vec{r} - (2\gamma) m \dot{\vec{r}}$$

Energy dissipation due to unspecified degrees of freedom

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14

Now, you may consider damping as well, and you know what damping is. So, damping off course is a result of you know energy loss it results in energy loss and one needs to know why there is the energy loss because in all the electromagnetic phenomenon are basically conservative interactions, and that is only interaction to consider, so why should there be an energy loss at all.

So, the energy loss actually comes only because when you set up your equation of motion you may not have taken into account in your equation of motion all the degrees of freedom. So, there will be some unspecified degrees of freedom due to which there is damping, and that will give you an a force which is proportional to the velocity and then there is an damping coefficient which is twice omega, so this is the usual classical description of damping.

(Refer Slide Time: 19:25)

atomic electrons 'driven' by Electric Intensity  
 Vector of EM field:  $\hat{\epsilon} E_0 e^{-i(\omega t + \theta)}$

**Damped + Driven oscillator**

$e$ : electron's charge

$$m \ddot{\vec{r}}(t) = -k\vec{r} - (2\gamma) m \dot{\vec{r}} + \hat{\epsilon} e E_0 e^{-i(\omega t + \theta)}$$

Driving force

$$m \ddot{\vec{r}}(t) = -\left(m\omega_{0,s}^2\right)\vec{r} - (\Gamma_d) m \dot{\vec{r}} + \hat{\epsilon} e E_0 e^{-i(\omega t + \theta)}$$

 PCD STAP Unit 7 Photoionization cross-section, pe angular distribution 15

And then you have this damped oscillator driven by this external field. So, you have got this natural restoring force minus  $k r$  there is this damping force, and then there is this driving force, so this is the equation of motion to damped driven classical oscillator. And this is the equation of motion which we need to solve and you would have done this in your classical mechanics course, or in electromagnetic theories. So, in number of different courses you meet this equation.

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$$m \ddot{\vec{r}}(t) + \Gamma_d m \dot{\vec{r}} + (m\omega_{0,s}^2) \vec{r} = \hat{\epsilon} e E_0 e^{-i(\omega t + \theta)}$$

$$\ddot{\vec{r}}(t) + \Gamma_d \dot{\vec{r}} + \omega_{0,s}^2 \vec{r} = \hat{\epsilon} \frac{e}{m} E_0 e^{-i(\omega t + \theta)}$$

Check:  $\vec{r}(t) = \hat{\epsilon} \frac{e}{m} \frac{E_0}{\omega_{0,s}^2 - \omega^2 - i\Gamma_d \omega} e^{-i(\omega t + \theta)}$  is a solution

$$\dot{\vec{r}}(t) = (-i\omega) \vec{r}(t)$$

$$\ddot{\vec{r}}(t) = (-i\omega)^2 \vec{r}(t) = -\omega^2 \vec{r}(t)$$

$$\left(-\omega^2 - i\Gamma_d \omega + \omega_{0,s}^2\right) \vec{r}(t) = \hat{\epsilon} \frac{e}{m} E_0 e^{-i(\omega t + \theta)}$$

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And if you divide by the mass you get this equation for the for the position vector, and it has got a solution which is well known, so this is the solution you can easily check it out you can get the velocity you can get the acceleration plug it in, and see for your cell very quickly. So, this is something that you would have done in your under graduate courses as well.

So, this is the usual solution to the damped driven classical oscillator. So, here omega is a frequency of the driving force and omega 0 comma s the natural frequency of the oscillator. So, these are the two frequencies that we are concerned with at this point, there is this damping coefficient gamma.

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$$(-\omega^2 - i\Gamma_d\omega + \omega_{0,s}^2)\vec{r}(t) = \hat{\epsilon} \frac{e}{m} E_0 e^{-i(\omega t + \theta)}$$

$$\vec{r}(t) \rightarrow 0 \text{ as } E_0 \rightarrow 0$$

Displacement of the electron from the equilibrium point is on account of the driving force and results in

**Induced** Oscillating Dipole Moment

**Classical Damped Oscillator**

Later, we connect Oscillator Strength to PI cross-section


PCD STAP Unit 7 Photoionization cross-section, pe angular distribution
17

And, you can easily see that this displacement of the electron goes to 0 as E 0 goes to 0. So, essentially we are talking about an induced effects, so we are talking about induced dipole moment. So, this induction is on account of the driving force which is why it is appropriate to talk about induced oscillating dipole moments, and this is the description that we get from classical oscillator.

So, this oscillator strength is what we need to be subsequently connected to the quantum mechanical transition probability and the photo ionization cross section, because when experimentalist talk about photoionization cross section they will always talk about you know how much oscillator strength is there under the photoionization curve, and that is where you really need to understand the term oscillator strength. So, that is part of the reason that we need to discuss spend some time discussing this classical model.

(Refer Slide Time: 22:06)

Connections:

- Oscillator Strength
- Atomic polarizabilities
- Photoionization cross-section



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So, these are the connections that we want to establish between oscillator strength atomic polarizabilities and the photoionization cross section.

(Refer Slide Time: 22:17)

$\alpha$ : atomic polarizability

$$\vec{d} = \alpha \vec{E} \quad \alpha = \frac{|\vec{d}|}{|\vec{E}|} \text{ induced dipole moment per unit electric field}$$

$$\vec{d} = e \vec{r}$$

$$\alpha = \frac{|\vec{e}\vec{r}|}{|\vec{E}|} = \frac{e \hat{\epsilon} \frac{E_0}{m \omega_{0,s}^2 - \omega^2 - i\Gamma_d \omega} e^{-i(\alpha t + \theta)}}{|\hat{\epsilon} E_0 e^{-i(\alpha t + \theta)}|}$$

$$\alpha = \frac{e^2}{m \omega_{0,s}^2 - \omega^2 - i\Gamma_d \omega}$$


PCD STIAP Unit 7 Photoionization cross-section, pe angular distribution 19

So, let me use the definition of atomic polarizability, so what is this, this is the induced dipole moment for unit electric field right. So, you have got a dipole moment you divided by the electric field which causes it, so the dipole moment is proportional to the electric intensity and the proportionality is given by what we call is the atomic polarizability. Now we also

know that the dipole moment is Harsh times displacement e into r, so these two are related they both describe the dipole moment. So, you can get alpha as the ratio of e r over E right.

So, you get alpha the atomic polarizability as the ratio of the dipole moment to the electric intensity and this, electric intensity you already know is the modulus of this applied electric field and the solution are is what we just obtained from the classical oscillator, which is the damped driven oscillator. So, the solution for r we already have with us, so we plug in this solution for r multiply it by this charge e and divided by the electric intensity, so this gives us the atomic polarizability.

So, now there is e square the other 2 places, where the electric charge comes, so you get e square over m. And if you take this modulus and divided by, this term over here you get omega 0 square minus omega square minus i gamma, so this is the complex number.

(Refer Slide Time: 24:20)

$\vec{d} = \alpha \vec{E}$  Atomic polarizabilities

$\alpha(\omega) = \frac{e^2}{m} \frac{1}{\omega_{0,s}^2 - \omega^2 - i\Gamma_d \omega}$   $\alpha = \frac{|\vec{d}|}{|\vec{E}|}$  induced dipole moment per unit electric field

$\alpha(\omega) = \frac{e^2}{m} \frac{1}{(\omega_{0,s} + \omega) \left[ (\omega_{0,s} - \omega) - i \frac{\Gamma_d \omega}{(\omega_{0,s} + \omega)} \right]}$

$\omega \approx \omega_{0,s}; \alpha(\omega) \approx \frac{e^2}{m} \frac{1}{2\omega_{0,s} \left[ (\omega_{0,s} - \omega) - i \frac{\Gamma_d \omega}{2\omega_{0,s}} \right]}$

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Alright now, in this complex number we have got omega 0 square minus omega square. So, this is like a square minus b square you can factor it as a plus b into a minus b and factor out this omega 0 plus omega is a common term. So, over here you have got omega 0 minus omega, but this term must be divided by omega zero plus omega. So, I only factored out this omega 0 plus omega 0 plus omega outside, but then the transition takes place at a frequency which is closest to the natural frequency.

So,  $\omega$  and  $\omega_0$  are very close to each other, within a certain width and you can therefore, represent this sum, as twice the natural frequency. Because, the sum of these 2 frequencies is hardly different from twice the natural frequency, but the difference of course you cannot ignore over here. Because, what you are ignoring is the small number compared to a large number you cannot ignore a small number, when you compare it with 0. So, here you retain the difference since  $\omega_0 - \omega$  but over here outside I have replaced this  $\omega_0 + \omega$  as twice  $\omega_0$ , which is twice the natural frequency.

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$$\alpha(\omega) = \frac{e^2}{m \omega_{0s}^2 - \omega^2 - i\Gamma_d \omega} \quad \therefore \alpha(\omega) \times \frac{m}{e^2} = \frac{1}{\omega_{0s}^2 - \omega^2 - i\Gamma_d \omega}$$

$$\text{now, } \vec{r}(t) = \hat{\epsilon} \frac{e}{m \omega_{0s}^2 - \omega^2 - i\Gamma_d \omega} E_0 e^{-i(\omega t + \theta)}$$

$$\therefore \vec{r}(t) = \hat{\epsilon} \frac{e}{m} \left[ \alpha(\omega) \frac{m}{e^2} \right] E_0 e^{-i(\omega t + \theta)}$$

$$\vec{r}(t) = \hat{\epsilon} \frac{E_0 \alpha(\omega)}{e} e^{-i(\omega t + \theta)}$$

**Dipole moment**

$$\vec{d}(t) = e \vec{r}(t) = \hat{\epsilon} E_0 \alpha(\omega) e^{-i(\omega t + \theta)}$$

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So, this gives me a fairly good approximation to the atomic polarizability, and if you just take this  $m$  cross multiply by  $m$  and  $e$  square, you get this term, which is very similar in its form to the solution to the displacement for the driven and damped oscillator. So, if you look at this similarity between these two forms, you can expect to write the displacement in terms of the polarizability, by factoring out the common terms because it has almost the same form.

And you write the displacement vector in terms of the polarizability, and this turns out to be  $e$  over  $m$  this is the direction of the polarization vector this is the frequency dependent polarizability, which is the complex number as we have seen then there is this  $m$  over  $e$  square which is coming from here. And there of course you have got the driving term. So, this is the solution to the displacement in terms of the atomic polarizability.

So, what is the dipole moment, it is just the charge times displacement, so you multiplied by this. So, this  $e$  cancels this  $e$  and you have got the rest of the terms here, there is an  $e$  in the denominator here.

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Average power pumped into the atomic system by the EM field is the real part of:

$$\langle Q \rangle = \frac{1}{T} \int_0^T \frac{dW}{dt} dt = \frac{1}{T} \int_0^T \vec{F} \cdot \vec{dr} dt$$

$$= \frac{1}{T} \int_0^T \left[ \left( \frac{\vec{F}}{e} \right) \cdot (e \dot{\vec{r}}) \right] dt$$

Concept of complex field is a mathematical tool.  
We are interested in its real part.....

Fano & Cooper Revs. Mod. Phys. July 1968 Section 2.1



PCD STAP Unit 7 Photoionization cross-section, pe angular distribution 22

So, this is what gives you the dipole moment, and now we ask what is the average power, which is pumped into the atomic system by the electronic field, and intuitively you should begin to expect that this will be related to the photoionization cross section. Because, our quantum mechanical object of interest is the transition probability, and that will be related to how much power is pumped into the atomic system by the electromagnetic field.

So, we first get a description of this quantity in terms of classical terms and classically this will be just the average of the rate of doing work right. So, if you  $dW$  by  $dt$  is a rate of doing work you integrate this over time and divide it by the periodic time, so that is the free corresponding to the frequency of oscillation. So, this will give you the average power over one period of the oscillation that an electromagnetic energy is pumped into the system, and this is off course a real quantity because physically you are dealing with real numbers.

So, this is the quantity that you want to get  $f \cdot dr$  is the work done. So, power is just the rate of change of the work done, so  $dW$  by  $dt$  is what you want to get. And if you divide  $f$  by  $e$  and multiply this by  $e$  you have got  $dr$  by  $dt$ , so you get  $f$  over  $e$  dot  $e$  time velocity, that is the term that you have to get and we have got these expressions from our classical oscillator. So, these quantities the way we have dealt with them are complex quantities we would we are

off course interested only the real part, which goes into the physical process; because power is a real physical quantity, so we will deal with the real parts.

(Refer Slide Time: 29:29)

Average power pumped into the atomic system by the EM field is the real part of:

$$\langle Q \rangle = \frac{1}{T} \int_0^T \frac{dW}{dt} dt = \frac{1}{T} \int_0^T \vec{F} \cdot \dot{\vec{r}} dt$$

$$= \frac{1}{T} \int_0^T \left[ \left( \frac{\vec{F}}{e} \right) \cdot (e \dot{\vec{r}}) \right] dt$$

Physical interest:  $\langle Q \rangle_{\text{Re}} = \frac{1}{T} \int_0^T \left[ \text{Re} \left( \frac{\vec{F}}{e} \right) \cdot \text{Re} (e \dot{\vec{r}}) \right] dt$

Real part



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So, this dot product that we have to work. With a flower  $e \dot{e} r \dot{r}$  you really need to take the dot product of the corresponding real parts and that will give you the physical power which is pumped in of interest. So, let us get this expression and evaluate it because we already have got expressions for dipole moment you have also have got the expression for the force.

(Refer Slide Time: 29:59)

$$\langle Q \rangle_{\text{Re}} = \frac{1}{T} \int_0^T \left[ \text{Re} \left( \frac{\vec{F}}{e} \right) \cdot \text{Re} (e \dot{\vec{r}}) \right] dt$$

$$\frac{\vec{F}}{e} = \hat{\epsilon} E_0 e^{-i(\omega t + \theta)}$$

$$\text{Re} \left( \frac{\vec{F}}{e} \right) = \hat{\epsilon} \frac{E_0}{2} \left[ e^{-i(\omega t + \theta)} + e^{+i(\omega t + \theta)} \right]$$

$$e \dot{\vec{r}}(t) = \hat{\epsilon} (-i\omega) E_0 \alpha(\omega) e^{-i(\omega t + \theta)}$$

$$\text{Re} [e \dot{\vec{r}}(t)] = \hat{\epsilon} \frac{E_0 \omega}{2} \left[ (-i)\alpha(\omega) e^{-i(\omega t + \theta)} + (+i)\alpha^*(\omega) e^{+i(\omega t + \theta)} \right]$$


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So, now  $f_e$  is the quantity here this is the electric intensity this is the force per unit charge, we need the real part which will be the cosine part of this, because the exponential function has got both the cosine and the sine part, the sine part comes with the imaginary  $i$  right. So, you take the  $e$  to the minus  $i$  theta and to the plus  $i$  theta divided by 2, so you will get half the cosine term, so this is the real part of the force per unit charge.

And likewise you need the real part of the dipole moment. So, here again you do the same thing and you have the dipole moment, which you had earlier described in terms of the complex atomic polarizability, you take this complex number multiply add to it, not multiply, but add to it the complex conjugate and then a divide by 2, so that will give you the real part of the dipole moment. So, now, we have got all the quantities of interest and now just you have to take the dot product of these two quantities.

(Refer Slide Time: 31:12)

$$\langle Q \rangle_{\text{Re}} = \frac{1}{T} \int_0^T \left[ \text{Re} \left( \frac{\vec{F}}{e} \right) \bullet \text{Re} (e \dot{\vec{r}}) \right] dt$$

The 'dot' product in the integrand:

$$\begin{cases} \hat{e} \frac{E_0}{2} [e^{-i(\omega t + \theta)} + e^{+i(\omega t + \theta)}] \\ \bullet \\ \hat{e} \frac{E_0 \omega}{2} [(-i)\alpha(\omega)e^{-i(\omega t + \theta)} + (+i)\alpha^*(\omega)e^{-i(\omega t + \theta)}] \end{cases}$$

$$= \frac{E_0^2 \omega}{4} \left[ \begin{aligned} &(-i)\alpha(\omega)e^{-i2(\omega t + \theta)} + (+i)\alpha^*(\omega) + \\ &(-i)\alpha(\omega) + (+i)\alpha^*(\omega)e^{+i2(\omega t + \theta)} \end{aligned} \right]$$

*What shall we get from the oscillatory functions over large time intervals?*

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So, let us do that you take the dot product of these two quantities in the integrand. So, it is the dot product of this quantity here, which is a real part of force per unit charge, this is the real part of the dipole moment, dotted out epsilon dot epsilon these are unit vectors that will give you unity. And then you have got this term into this term which will give you  $e$  to the minus twice this phase angle.

When you take the product of this term and this term the  $e$  to the minus  $i$  theta and  $e$  to the plus  $i$  theta will cancel. So, you get  $i$  times alpha star omega, so likewise you will have a minus  $i$  times alpha omega coming from here from these two terms comes; and then again

form the last two terms you get from this term and this term you get a plus twice I the phase right. So, now we will be interested in carrying out observations over long intervals of time and we should ask what is it that this will lead to over as we integrate this quantity over large intervals of time.

(Refer Slide Time: 32:27)

$\langle Q \rangle_{Re} = \frac{1}{T} \int_0^T \left[ \text{Re} \left( \frac{\vec{F}}{e} \right) \cdot \text{Re} (e \dot{r}) \right] dt$

The 'dot' product in the integrand:  $= \frac{E_0^2 \omega}{4} \left[ \begin{matrix} (-i)\alpha(\omega)e^{-i2(\omega t + \theta)} + (+i)\alpha^*(\omega)e^{+i2(\omega t + \theta)} \\ (-i)\alpha(\omega) + (+i)\alpha^*(\omega)e^{+i2(\omega t + \theta)} \end{matrix} \right]$

$\int_{t \rightarrow -\infty}^{t \rightarrow \infty} e^{\mp i2(\omega t + \theta)} dt = ?$  ; For large  $t$  ( $E_0 = 0$  for  $t < 0$ )  
so the range of integration  $-\infty \rightarrow 0$  included)

$\int_{t \rightarrow -\infty}^{t \rightarrow \infty} e^{\mp i2(\omega t + \theta)} dt = \pm \frac{\pi}{2} \delta(\omega) \quad \omega = 0 \rightarrow$   
*no oscillations*


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26

So, what is the integral of this  $e$  to the minus  $i$  to a phase factor here because this is this is the only time dependent function which is coming here right. So, over integrals over time, the integration of course has to be carried out from, the instant that photo absorption takes place. So, integration is from 0 to infinity, let say for large time I will say  $t$  ten into infinity, so your integration range is from 0 to infinity, but mind you all of these quantities are multiplied by  $e_0$ , but  $e_0$  was 0 before  $t$  equal to 0 right there was no electric field which was applied.

So, without any loss of generality I can extend the range of integration from minus infinity to plus infinity giving me the same result, because you are adding a number of 0 to the result. So, it really does not matter, but the advantage is that by extending the range of integration from minus infinity to plus infinity you recognize that you get a delta function, so that gives you a very simple result. And the delta function whose argument is a frequency will contribute to the integrals only when  $\omega$  is equal to 0, and  $\omega$  is equal to 0 corresponds to no oscillation right, so that is not going to contribute anything to the oscillatory part at all.

(Refer Slide Time: 34:19)

$$\langle Q \rangle_{\text{Re}} = \frac{1}{T} \int_0^T \left[ \text{Re} \left( \frac{\vec{F}}{e} \right) \bullet \text{Re} (e \dot{\vec{r}}) \right] dt$$

The integrand:  $= \omega \frac{E_0^2}{4} \left[ (+i)\alpha^*(\omega) + (-i)\alpha(\omega) \right]$

$$\alpha = a + ib$$
$$(+i)\alpha^*(\omega) + (-i)\alpha(\omega)$$
$$= (+i)(a - ib) + (-i)(a + ib)$$
$$= +b + b = +2b = 2 \text{Im} \alpha(\omega)$$


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27

So, the quantities of interest therefore, which we will be concerned with are those which are inside these red boxes because these will make low contribution. So, the physical phenomenon in which we are interested. So, mathematically you get these terms these oscillatory terms, but they are of no interest for the physical processing of this information, see you have got only these two terms in these red boxes.

So, those are the ones which I have written here, and alpha is some complex number, so you have got i times alpha star and you have to subtract from that minus, i times alpha which is the complex conjugate of this. So, initially what you get when you do this summation is twice the imaginary part of alpha; what does it mean we really arrive at an extremely simple, but a very important result which is the following.

(Refer Slide Time: 34:52)

Average power pumped into the atomic system by the EM field is given by:

$$\langle Q \rangle_{\text{Re}} = \frac{1}{T} \int_0^T \left[ \text{Re} \left( \frac{\vec{F}}{e} \right) \cdot \text{Re} (e \dot{\vec{r}}) \right] dt = \frac{\omega E_0^2}{2} \text{Im} \alpha(\omega)$$

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28

That the average power which is pumped into the atomic system by their electromagnetic field is given by  $\omega e_0^2$  square by 2. You remember where this  $\omega e_0^2$  square by 2 is coming from.

(Refer Slide Time: 35:04)

$$\langle Q \rangle_{\text{Re}} = \frac{1}{T} \int_0^T \left[ \text{Re} \left( \frac{\vec{F}}{e} \right) \cdot \text{Re} (e \dot{\vec{r}}) \right] dt$$

The integrand:  $= \omega \frac{E_0^2}{4} [(+i)\alpha^*(\omega) + (-i)\alpha(\omega)]$

$\alpha = a + ib$

$(+i)\alpha^*(\omega) + (-i)\alpha(\omega)$

$= (+i)(a - ib) + (-i)(a + ib)$

$= +b + b = +2b = 2 \text{Im} \alpha(\omega)$



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27

It is coming from here, this is  $\omega e_0^2$  square by 4, but then there is a twice a imaginary part of alpha. So, this 2 and this 1 over 4 is what gives you the 1 over 2, so  $\omega e_0^2$  square by 2 is what you get times, the imaginary part of the complex atomic polarizability.

(Refer Slide Time: 35:28)

Average power pumped into the atomic system by the EM field is given by:

$$\langle Q \rangle_{\text{Re}} = \frac{1}{T} \int_0^T \left[ \text{Re} \left( \frac{\vec{F}}{e} \right) \cdot \text{Re} (e \dot{\vec{r}}) \right] dt = \frac{\omega E_0^2}{2} \text{Im} \alpha(\omega)$$

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And this is a result which you will find in Fano and Cooper's paper you will find it in Fano and Rao's book, and in a lot of literature on atomic photo absorption processes in which, they will relate the photoionization cross section and tell you that it is a measure of the imaginary part of the atomic polarizability, and this is the connection which I wanted to established in today's class.

So, it is essentially a classical model that, I wanted to discuss today and in the next class I will introduce the quantum mechanical treatment. So, I will off course be defining what is called as the oscillator strength in a rigorous manner, but that is something I would do in the next class. So, if there are any questions I will be happy to take.

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Average power pumped into the atomic system by the EM field is given by:

$$\langle Q \rangle_{\text{Re}} = \frac{1}{T} \int_0^T \left[ \text{Re} \left( \frac{\vec{F}}{e} \right) \cdot \text{Re} (e \dot{\vec{r}}) \right] dt = \frac{\omega E_0^2}{2} \text{Im} \alpha(\omega)$$

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28

Yes on any part of the class, if none.

Thank you very much.