Original Research Article

Angular distribution of atomic photoelectrons as a function of photon field polarization: Case of ns-type light atoms

Abstract

The angular distribution of the cross section of the photoelectrons of an atom, gives us information on the evolution of field of the photoelectrons in different directions, with respect to the incident direction of the electromagnetic radiation which is absorbed by the atom and its direction of polarization. Here, the angular distribution of atomic photoelectrons as a function of photon field polarization was studied theoretically using monocentric wave functions to investigate the influence of polarization on the theoretical results. A GEANT4 modeling calculation based on the Monte Carlo code was made on the helium atom. The calculations were performed at low energy above the atomic ionization threshold. The results obtained by analytical calculation for the total photoionization cross section were compared with those obtained by a simulation calculation using GEANT4 modelling.

Keywords: *Angular distribution, Cross-Section, Photoelectron, Polarization. GEANT4*

I. INTRODUCTION

The angular distribution of atomic photoelectrons has been the subject of constant study, both theoretical and experimental [8-14]. It is therefore useful to study the influence of polarization of the electric field of the wave on the angular distribution of atomic photoelectrons for an energy range above the ionization threshold of an atom. In a photon collision, a photon of energy collides with an atomic or molecular target. During this process, two types of collisions can take place: elastic and inelastic. In the elastic case, the final state is composed of the same particles as the initial state (the internal state of the particles remains unchanged):

$$h\nu + A \rightarrow h\nu' + A'$$

While in the inelastic process, the photon transfers part of its kinetic energy to the target which results, either in an excitation, or in a photoionization of the atom:

$$h\nu + A \rightarrow A^{+} + e^{-}$$

In this study, only the process of simple photoionization of the atom will be considered, the aim of which will first be to study the angular distribution of the probability of ionization of an atom at a given energy as a function of the polarization of the field electric of the electromagnetic wave. Then, it will be made case of application to light atoms of ns types. In this article, we study the angular distribution of photoelectrons of an atom at the ionization threshold as a function of the polarization of the electric field of the electromagnetic wave.

The model used consists in dealing with the problem using the dipole approximation using monocentric wave functions describing the bound states of the atom of interest. The ejected electron will be described by a Coulomb wave taking into account the interaction between this electron and the residual ion. The projectile is itself described by a plane wave.

In the part entitled theory and method of calculation, a brief outline on the theory of the angular distribution of the photoelectrons as well as the methods of calculation were exposed. The results and discussions part provides the theoretical results on the one hand and a comparison between the calculation of the theoretical total cross section of the helium atom and the result of the calculation obtained by geant4 simulation on

the other hand. And finally, a brief discussion of the results will ensue.

II. THEORY AND METHOD OF CALCULATION

The object of this present work to study the process $(h\nu;e)$ in the case of atomic target A . A polarized photon, with energy greater than the ionization threshold I I_p tears an electron from an atom A:

$$h\nu + A(0,0) \rightarrow A^{+}(L_i, M_i) + e^{-}(l,m) \quad (1)$$

Where the incident photon has for wave vector $\vec{k}$, the ejected photoelectron with wave vector $\vec{k}_f$ is identified by its coordinates r. From an experimental point of view, the vector $\vec{k}_f$ defines the direction of detection of the ejected photoelectron. Where magnetic quantum numbers refer to a quantization axis parallel to the direction of polarization. For this process to occur, the photon energy must be equal to or greater than the threshold energy or ionization potential I_P. The electron is ejected with kinetic energy. $E_C = h\nu - I_P$.

II.1. The initial state of the system:

In the initial state, the system consists of an atomic target A and an incident photon described by a plane wave. o describe the bound states of the atomic target, monocentric wave functions are used. We neglect the delay effects resulting from the dynamics of the photon [5]. The initial state of the atom is in a defined state of angular momentum and can be represented by: $|\psi_i\rangle = R_{n,l'}(r)|l', m'\rangle$ (2)

where $R_{n,l'}(r)$ gives the radial behavior of the wave function..

II.2. The final state of the system :

The final state of the system is composed of an ejected photoelectron e^{-} of momentum $\vec{k}_f$, and an atomic ion A^{+}. Using the active one-electron model, the continuum state of the atom must have the correct asymptotic form a plane wave as well as incoming spherical waves [5]. If $\vec{k}$ is a unit vector along the outgoing electron ejection direction, we can write:

$$|\psi_f\rangle = \psi_{\vec{k}}^{(-)} = 4\pi \sum_{l,m} (i)^l e^{-i\delta_l} Y_{l,\mathrm{m}}^{*}(\hat{k}) Y_{l,m}(\hat{r}) G_{k,l}(r) \quad (3)$$

Where $G_{kl}(r)$ is the radial wave function divided by kr and δ_l is the phase shift of the scattered partial wave l .

II.3. Expression of the absorption cross section of a photon in dipole approximation

In dipole approximation, the absorption cross section of a photon with energy $h\nu$ by a free atom which passes from an initial state written by the wave function ψ_i to a final state written by the wave function ψ_f (wave function of the system consisting of a positive ion and the ejected electron with a kinetic energy T) is written [1]:

$$\sigma(h\nu) = \frac{P_{if}}{F}. \quad (4)$$

where, $h\nu = I_P + T$ (I_P is the photon energy for which the electron is released with zero kinetic energy) ;

$$P_{if} = \frac{2\pi}{\hbar} \left| \langle \psi_f | \frac{e\hbar}{2imc} \vec{A}_0 \cdot e^{i\vec{k}\vec{r}} \cdot \vec{\nabla} | \psi_i \rangle \right|^2 \delta(\tilde{\omega})$$

(5), is the transition probability per unit time;

$F = \frac{A_0^2}{8\pi} \frac{\omega}{\hbar c}$ (6), is the flux of the incident photon calculated from the intensity of the pointing vector where is the amplitude of the wave. Let the one-photon differential cross section be [1]:

$$\sigma(h\nu) = \frac{4\pi^2 \alpha \hbar^2}{m^2 \omega} \times \left| \langle f | e^{i\vec{k}\bullet\vec{r}} \hat{\varepsilon} \bullet \vec{\nabla} | i \rangle \right|^2 \times \delta(\tilde{\omega}). \quad (7)$$

Where $\tilde{\omega} = \omega - \omega_{fi}$; ∇ is the component along the direction of polarization x of photon of the vector $\vec{\nabla}$, with $\vec{\nabla} = \frac{i}{\hbar}\vec{p}_{fi} = \frac{im}{\hbar}\vec{v}_{fi} = \frac{m}{\hbar} w_{fi} \vec{r}_{fi}$ (8) , and α is the fine structure constant. The vectors $\vec{p}$,

$\vec{v}$, $\vec{r}$, being respectively the operators total linear momentum, total velocity and sum of the radii vectors of the electrons. But, $\vec{\varepsilon}\cdot\vec{\nabla}=\vec{\varepsilon}\cdot\frac{i}{\hbar}\vec{p}_{fi}=\vec{\varepsilon}\cdot\frac{im}{\hbar}\vec{v}_{fi}=\frac{imI_p}{\hbar^2}\vec{\varepsilon}\cdot\vec{r}$ with $I_P=\hbar w_{fi}=E_i-E_f$.

So the equation (7) becomes:

$$\sigma(h\nu)=\frac{4\pi^2\alpha I_P^2}{\hbar^2\omega}\left[\left\langle\psi_f\left|T\right|\psi_i\right\rangle\right]^2\delta(\tilde{\omega}) \quad (9)$$

Where $T=e^{i\vec{k}\cdot\vec{r}}\vec{\varepsilon}\cdot\vec{r}$, is the transition operator. In this expression of $\sigma(h\nu)$ we did not take into account the spin of the electron and we limited ourselves to the non-relativistic dipole approximation. The transition matrix element M of the previous equation is the following:

$$M=\left\langle\psi_f\left|e^{i\vec{k}\cdot\vec{r}}\vec{\varepsilon}\cdot\vec{r}\right|\psi_i\right\rangle=\left\langle\psi_f\left|\vec{\varepsilon}\cdot\vec{r}\right|\psi_i\right\rangle . \quad (10)$$

(With $e^{i\vec{k}\cdot\vec{r}}\approx 1$ dipole approximation).

II.4. Calculation of the transition matrix element : $\left\langle\psi_f\left|\vec{\varepsilon}\cdot\vec{r}\right|\psi_i\right\rangle$

Here we have used the 3-j Wigner symbols and some spherical harmonic identities to calculate the transition matrix element as a function of the electric field polarization of the wave assuming that the field polarization associated with the photon:

II.4.1. is linear to lead to the expression of the transition matrix element in the form:

$$\left\langle\psi_f\left|rC_0^1\right|\psi_i\right\rangle=\sum_{l,m}a(l,m)(-1)^{l-m+g}l_{\succ}^{\frac{1}{2}}\sigma_l\begin{pmatrix}l & 1 & l'\\ -m & 0 & m'\end{pmatrix} \quad (11)$$

II.4.2. is circular to result in the expression of the transition matrix element as:

$$\left\langle\psi_f\left|rC_1^1\right|\psi_i\right\rangle=\sum_{l,m}a(l,m)(-1)^{g'}l_{\succ}^{\frac{1}{2}}\sigma_l\begin{pmatrix}l & 1 & l'\\ -m & 1 & m'\end{pmatrix} \quad (12)$$

Where $a(l,m)=4\pi(i)^l e^{-i\delta_l}Y_{l,m}^*\left(\hat{k}\right)$; $l_{\succ}$ is the maximum value of l and l' ; σ_l is the integral dipole; $g=\frac{l'-l+1}{2}$; and $g'=\frac{l'+l+1}{2}$.

So in these two cases of photon polarization, the matrix element is an integral over the radial and angular variables.

In this study, we had made linear and circular case of the polarization of the photon by limiting ourselves to the dipolar approximation. The latter, although it has its limits [10-11], is a good approximation for an energy range below 1.keV [7].

II.5.1. Linear polarization of the photon

In the dipole approximation, the differential cross section of the ejected photoelectrons for a linear polarization of the photon is:

$$\sigma(h\nu)=\frac{\sigma_{total}}{4\pi}\left[1+\beta P_2(\cos\theta)\right]. \quad (13)$$

II.5. Angular distribution of the photoelectrons

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

is the asymmetry parameter, and $P_2(\cos\theta)=\frac{3\cos^2\theta-1}{2}$ is the Legendre polynomial of order 2, θ is the angle between the direction of emission of the photoelectron and the polarization of the photon,

$$\sigma_{total} = \frac{64\pi^3 \alpha \left(E_i - E_f\right)^2 \left[l\sigma_{l-1}^2 + (l+1)\sigma_{l+1}^2 \right]}{3\omega\hbar^2 (2l+1)}$$

is the total photoionization cross section, σ_l is the integral dipole. The β parameter depends on the atom considered and varies between -1 and +2. Whatever the β value of the angular distributions of the photoelectrons have a symmetry of revolution around the polarization of the photon.

II.5.2. Circular polarization of the photon

For circularly polarized light, the angular distribution of photoelectrons can be written in the following form:

$$\sigma(h\nu) = \frac{\sigma_{total}}{8\pi}\left[1 + \beta P_2(\cos\theta) + a + b\cos^2\theta\right] \quad (14)$$

Where $a = 3 \cdot \frac{l^2\sigma_{l-1}^2 + (l+1)^2\sigma_{l+1}^2}{l\sigma_{l-1}^2 + (l+1)\sigma_{l+1}^2}$, and

$b = -3 \cdot \frac{l(l-1)\sigma_{l-1}^2 + (l+1)(l+2)\sigma_{l+1}^2}{l\sigma_{l-1}^2 + (l+1)\sigma_{l+1}^2}$ are parameters expressed as a function of integral dipole for the orbital moment $l' = l \pm 1$. Much more information on the total cross section is given by [12-13].

II.5.3. Calculation of the simulation

The simulation part of the calculation briefly illustrates the simulation technique carried out for the numerical compilation of the interaction cross sections. First of all, for the compilation of the differential cross sections of the ns-type light atoms, the plot of the angular distribution of the photoelectrons was carried out using the MATLAB software to clearly highlight the influence of polarization on the types of polarizations considered in this study. MATLAB is a scripting language emulated by a development environment of the same name. It is used for numerical calculation purposes and graphical visualization. Then, with regard to the energy distribution of the ejected photoelectrons as well as the total cross section of atomic photoionization, the modeling was carried out with the GEANT4 tool based on Monte Carlo code [15]. The latter is free software that allows you to accurately simulate the passage of particles through matter. Full information about Geant4 is available online. Four documents of interest for users can be cited: the geant4 source code; the GEANT4 installation guide [6]; the Application Developers Guide [2] and the Physics Reference Manual [9]. In this model, the target is represented by a homogeneous cube filled with helium (gas), the primary projectile is a point source of the energy photon $h\nu$ fired at the center of the target. The physical processes considered in this GEANT4 simulation model are: standard electromagnetic processes; Penelope physics and Livermore physics. Then, the output and the analysis of the results were carried out using the ROOT software. The latter is a program specially designed for the analysis of data in particle physics. It was created in the 90s at CERN. ROOT is a class library available for free and easy to install on most machines.

III. RESULTS AND DISCUSSIONS

III.1. Case of light atoms

For ns-type light atoms, the orbital moment $l = 0$ and the asymmetry parameter β is equal to 2. So theoretically, the angular distribution of the photoelectron of ns-type light atoms is in $\cos^2\theta$ in the linear case of photon polarization and in $\sin^2(\theta)$ for circularly polarized light. For some values of the energy of the incident photon, one obtains the graphs of the angular distributions of the photoelectrons according to the angle θ of ejection which varies from **0** to π.

III.1.1. Linear case of photon field polarization

$$\sigma(h\nu) = \frac{3\sigma_{total}}{4\pi}\cos^2(\theta)$$

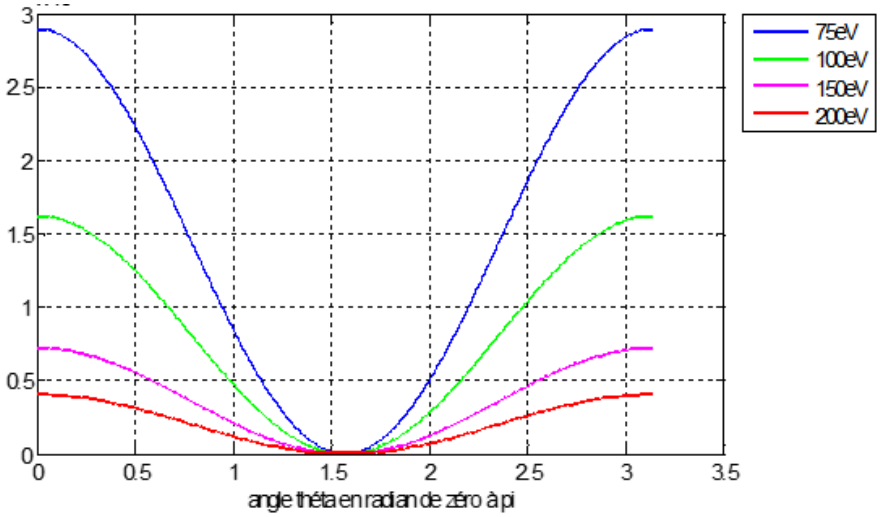

Figure 1: Curves of the photoelectron angular distribution as a function of the ejection angle θ for a linear polarization of the photon (case of ns-type light atoms)

III.1.2. Circular case of photon field polarization

$$\sigma(h\nu) = \frac{3\sigma_{total}}{8\pi}\sin^2(\theta)$$

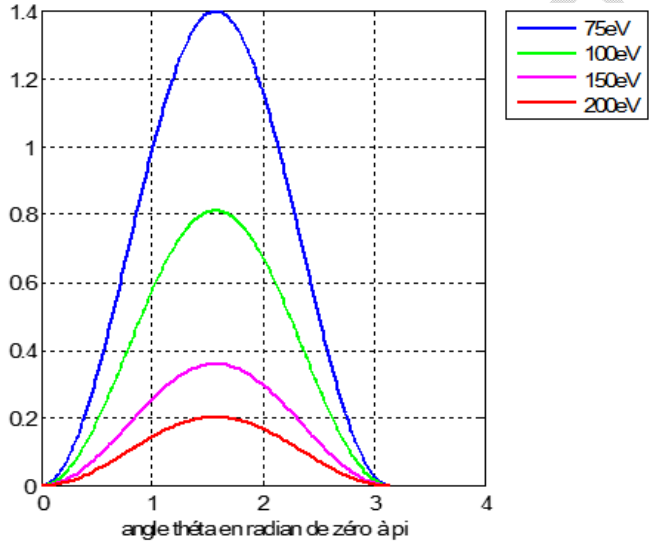

Figure 2: Curves of the photoelectron angular distribution as a function of the ejection Angle θ for a circular polarization of the photon (case of ns-type light atoms).

III.1.3. Influence of polarization

$$\sigma_{cir}(h\nu,\theta) = \frac{1}{2}\sigma_{lin}\left(h\nu,\left(\theta - \frac{\pi}{2}\right)\right)$$

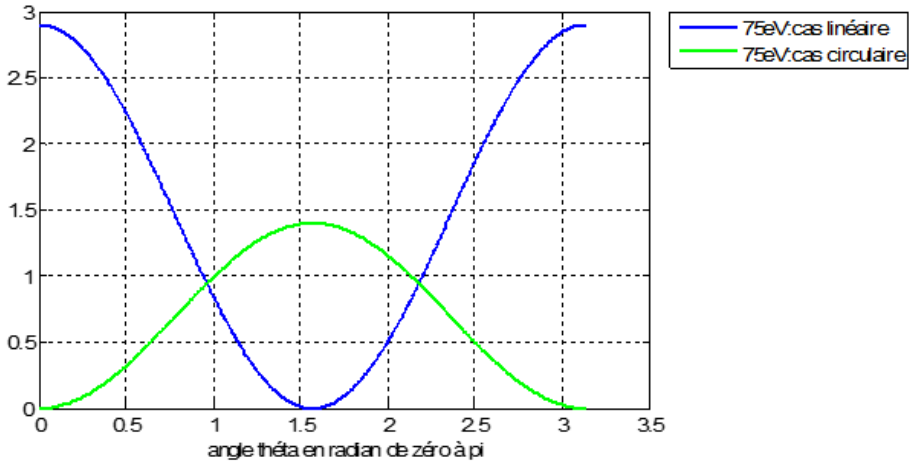

Figure 3: Curves of superposition of the angular distribution of photoelectron in the two cases of polarization $h\nu = 75eV$

III.2. Application to the helium atom

The helium atom is the simplest two-electron system, it is a chemical element belonging to the family of noble gases, that means, it does not react with other species except at rare exceptions. The primary kinematics is a source of the photon fired at the center of a simple box filled with helium gas.

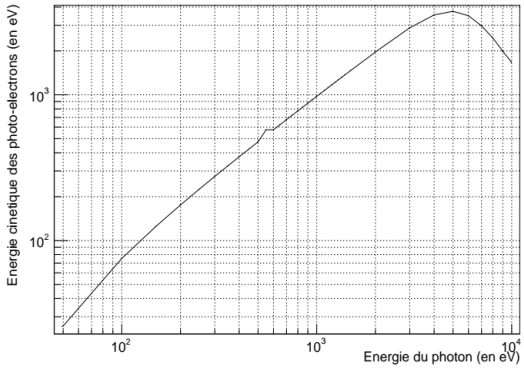

Figure 4: Energy distribution of the photoelectrons of a helium atom as a function of the energy of the incident photon: GEANT4 simulation

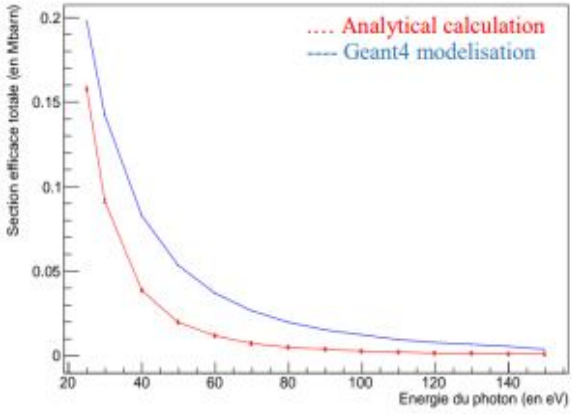

Figure 5: Total photoionization cross section of the helium atom: Comparison between theory (dotted red curve) and GEANT4 simulation (blue curve).

Figures 1.2 give the variation of the angular distribution of the differential cross section as a function of the ejection angle of the photoelectrons but also as a function of the energy of the incident photon where we note that the total cross section decreases with the energy of the incident photon. This decrease is explained by the fact that theoretically in the case of polarized light, the total cross section is inversely proportional to the square of the energy of the incident photon. In ***figure1*** corresponding to the linear case of polarization of the photon, the photoelectrons are more ejected towards the front and the back of the incident plane. In the case of a circular polarization, figure 2, the photoelectrons are preferentially ejected perpendicular to the plane of incidence. By observing the curves of ***figure 3***, one would notice on the one hand that these two curves are out of phase with the

wave and that the amplitude of the curve of the angular distribution in the circular case measures half of that in the case linear polarization of the photon. The observed phase shift is explained by the fact that in practice, circularly polarized light is obtained from linearly polarized light by passing it through a plate lagging a quarter wave with its axes at 45 degrees from relative to its axis of polarization. From the energy point of view, in the case of a circularly polarized wave, the energy of the incident photon breaks down into two waves of the same energy intensity, polarized along ***x*** and ***y*** for example, while in the linear case of polarization of the photon, the incident electromagnetic radiation is entirely polarized in a single direction ***x*** for example. It emerged from this study that in the linear case of photon polarization, unlike the circular case, the maximum signal (peak) is obtained when the ejection angle of a photoelectron $\theta = 0$ (ejection of electron towards front) or $\theta = \pi$ (backscatter).

Figure4 gives us the energy distribution of the photoelectrons of the helium atom as a function of the energy of the incident photon. That is, the average kinetic energy with which the photoelectron is ejected from the atomic target during the interaction between a photon is an atomic target. The kinetic energy of the photoelectron increases with the energy of the incident photon up to a certain value of the energy of the photon around ***5keV*** where the photoelectron acquires a maximum kinetic energy equal to approximately ***3.742keV***. Therefore, from a certain value of the energy of the photon (approximately ***5keV***) in interaction with a volume of helium, the absorption is no longer total because from this limit value, part of the incident photons comes out of the interaction medium without interacting with the target at all. ***Figure 5*** provides a comparison of the total photoionization cross section of the helium atom between the analytical calculation and that obtained by GEANT4 simulation based on the Monte Carlos code of particle transport. The dotted curve in red color gives the analytical total cross section of the helium atom in the dipole approximation and the curve in blue color gives the result of a modeling of the total cross section of the helium atom obtained by GEANT4 simulation. Although there is a considerable discrepancy in the total cross section of the helium atom between the analytical compilation and the GEANT4 modeling at the helium ionization threshold , we note that these two curves approach each other for a photon energy well above the ionization threshold of this atom considered. This difference can be explained by the fact that by analytical calculation, the cross section relating to the photoelectric effect cannot be expressed without resorting to mathematical approximations whereas the GEANT4 modeling takes into account the global parameters for the calculation total cross section of the photoelectric effect [16]. The dipole approximation although it has its limits, is therefore a good approximation at low energy.

IV. CONCLUSION

During this study, the angular distribution of photoelectrons in the linear and circular case of photon field polarization was calculated. Then an application to light atoms of the ns type was carried out in order to draw the influence of the polarization on the results of these two polarizations. Then a numerical simulation calculation using the geant4 software was particularly carried out on the helium atom. This calculation allowed us to compare the total cross section of the helium atom between the results of an analytical calculation and those obtained by GEANT4 simulation based on the (Monte Carlos) particle transport code.

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