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Two Photon Atomic Processes

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1 Introduction

Both inelastic and elastic two photon atomic processes allows to investigate the structure of atoms. We mention Raman and anti-Raman scattering as inelastic processes when both final and initial states are bounded states as well as Compton scattering when the final state of the electron belongs to the continuum spectrum of the energy. A correct calculation of a Compton profile gives the right electron momentum distribution in atom. Elastically scattered photons by bound electrons (Rayleigh scattering) are used extensively for determining the composition and structure of materials. Due to the development of high intensity X-ray and gamma-ray sources, Rayleigh scattering both above and below the photoeffect threshold energy has become a standard tool for studying the structure and properties of various materials involving intermediate and high atomic numbers. The Rayleigh scattering is also of great interest for the investigation of scattering processes from the atomic ground state nanometric powders, amorphous materials and dilute media , flames, ionized gases and plasma, optical properties of fibers, and many other fields. We consider that the photon energy range of interest lies from a few hundred eV up to 300 KeV and in this energy range scattering must be described with quantum theory. When investigating the interactions of the electromagnetic field with the inner shells electrons of high Z atoms, the incident photons energies are in the X and gamma-ray domain, so that accurate analytical formulae are needed for this range of energies. The atomic model considers that independent atomic electrons interact with a single screened central potential resulting from the charge distribution of the nucleus and all the atomic electrons.

Elastic scattering of photons by the atom is considered as elastic scattering by the bound electrons and nucleus which in the final state remain bound. Because the energy of the scattered photon is the same as that of the incident photon, it is impossible to distinguish which of the atomic component is responsible for the scattering. Hence, in order to obtain the scattering cross section we must sum the scattering amplitudes of the atomic components (electrons and nucleus) and only then squares. That means that we have to consider a coherent sum of the amplitudes. By Rayleigh scattering we mean the contribution made to elastic scattering by the atomic electrons-an atomic process. Elastic scattering by the nucleus includes nuclear Thomson scattering (scattering by the charge of the nucleus), Delbruck scattering (a radiative correction to nuclear Thomson scattering and a nonclassical, nonlinear interaction of the electromagnetic fields), and nuclear resonance scattering.

In the nonrelativistic approach, a two photons process in the lowest orders of the perturbation theory is described by the Kramers-Heisenberg-Waller (KHW) matrix element [1,2]

$$\begin{aligned} M_{KHW} = & \left(\vec{s_1}\,\vec{s_2}\right)\left\langle f|e^{i(\vec{k_1}-\vec{k_2})\,\vec{r}}\,|i\right\rangle - \\ & - \langle f|\,e^{-i\,\vec{k_2}\,\vec{r_2}}\left(\vec{s_2}\,\vec{P_2}\right)\,G_0^{NR}\left(\vec{r_2},\vec{r_1};\Omega_1\right)e^{i\,\vec{k_1}\,\vec{r_1}}\left(\vec{s_1}\,\vec{P_1}\right)|i\rangle - \\ & - \langle f|e^{i\,\vec{k_1}\,\vec{r_2}}\left(\vec{s_1}\,\vec{P_2}\right)\,G_0^{NR}\left(\vec{r_2},\vec{r_1};\Omega_2\right)e^{-i\,\vec{k_2}\,\vec{r_1}}\,|i\rangle \end{aligned} \tag{1.1}$$

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where $\vec{k_1}$ and $\vec{k_2}$ are the momentum vectors of the incident and scattered photon and $\vec{s_1}$ and $\vec{s_2}$ are the polarization vectors of the incident and scattered photons. In the KHW matrix element $\Omega_1 = \omega_1 + I_B$, $\Omega_2 = -\omega_2 + I_B$, where ω_1 and ω_2 stand for the energy of the incoming and scattered photon respectively, and I_B is the ionization energy of the electron. In the equation (1.1) the states $|f\rangle$ and $|i\rangle$ are solutions of the Schrdinger equation with Coulomb field. The sum over the complete set of intermediate states may be replaced by the coulombian nonrelativistic Green function defined as

$$G_0^{NR}(\vec{r_2}, \vec{r_1}; \Omega) = \underset{n}{S} \frac{u_n(\vec{r_1}) u_n^*(\vec{r_2})}{E_n - \Omega}, \tag{1.2}$$

or

$$(H_0 - \Omega)\ G_0^{NR}\left(\vec{r_2}, \vec{r_1}; \Omega\right) = \delta\left(\vec{r_2} - \vec{r_1}\right) with\ H_0 = \frac{\vec{P}^2}{2m} - \frac{\alpha Z}{r} \tag{1.3}$$

It may be shown that the nonrelativistic coulombian Green function depends on two parameters,

$$X^2 = -2m\Omega, ReX > 0\ and \tau = \alpha Z m / X \tag{1.4}$$

the relationships between parameters being given by nonrelativistic kinematics.

The first term of the equation (1.1) is the nonrelativistic form factor coming from the $\vec{A}\,2$ term of the Hamiltonian for the interaction of the radiation field with an electron

$$H_{\text{int}}^{NR} = \frac{e^2 \vec{A}\,2}{2m^2} - \frac{e}{m} \vec{A}\,\vec{P}\ ,$$

while the matrix elements involving the coulombian Green function come from the linear term in the potential $\vec{A}$ from the operator H_{int}^{NR}.

The exponential function present in the KHW matrix element gives the multipole and retardation contributions. We notice that by retarded contributions is meant the evaluation of multipoles beyond their long wavelength limit. Some time ago Costescu et al [3] have shown in the case of Rayleigh scattering, that multipole and retardation corrections are important and significantly larger than relativistic correction for photon energies ω above the K-shell photo-effect threshold I_B, but far enough from spurious poles which occur in the nonrelativistic fully retarded amplitude. For photon energies above 50 keV the contributions from spurious poles near the electron-positron pair production threshold [3, 4] in the Rayleigh nonrelativistic retarded amplitude, degrade the predicted numerical results, largely overestimating the elastic photon scattering and photoeffect cross-sections. The effects of these poles are known in photoeffect (which is related to the imaginary part of the forward Rayleigh scattering amplitude by the optical theorem).

The nonrelativistic result including all multipoles and retardation was obtained by Fischer [5]. It may be written

$$\sigma_{\text{ph}} = \frac{32\pi^2}{3\alpha} r_0^2 (\alpha\ Z)^6 \left(\frac{m}{\omega}\right)^4 \frac{e^{-2|\tau_1|\chi(k_{\text{NR}}, Z)}}{1 - e^{-2\pi|\tau_1|}} \frac{1}{\left[(1 - \omega/2m)^2 + \alpha^2 Z^2\right]^2} \tag{1.5}$$

where

$$\chi = \arctan \frac{2(k+1)^{1/2}}{2 - k + (k\alpha Z/2)^2}$$

It is obvious that Fischer's cross-section presents spurious poles located at $\omega = 2m \pm i2\alpha Z m$.

The poles near the pair production threshold in this nonrelativistic retarded result cause substantial departures from the nonretarded dipole result at high energies, where the nonretarded dipole result is known to agree with calculations including retardation and relativity, implying a cancelation of these poles by relativistic contributions. This observation applies to both screened and Coulombic calculations of the total photoeffect cross section.

Recently, it has been proven [6] that in the case of Compton scattering on K-shell bound electrons the nonrelativistic KHW matrix element leads to inadequate expressions for the nonrelativistic Compton amplitudes when the sum over the complete set of positive-energy intermediate states is replaced

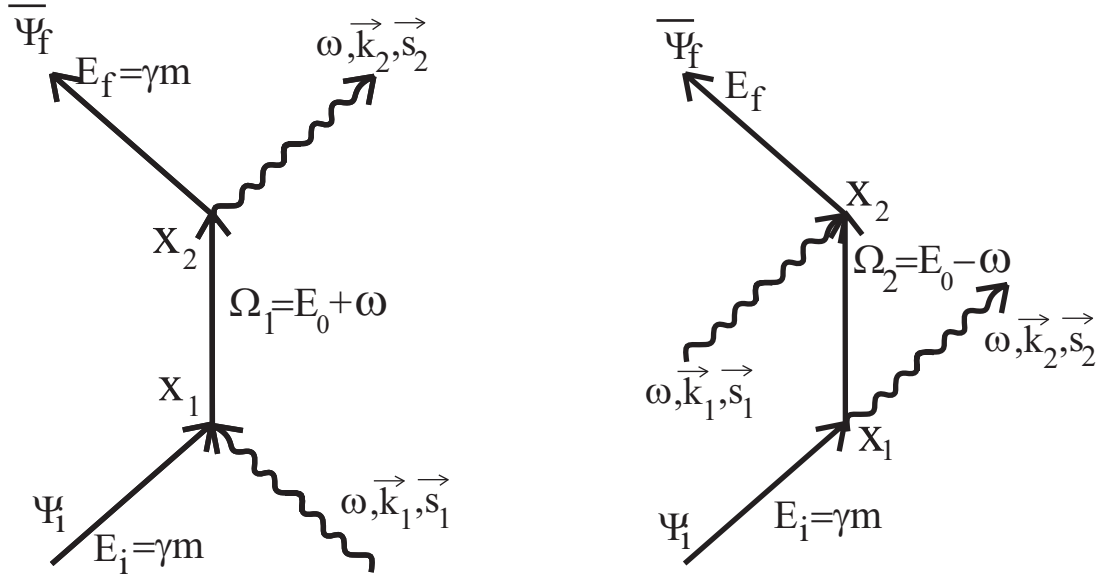

Figure 1: Feynman diagrams for the second order amplitudes of the two photon scattering.

by the integral representation of the nonrelativistic coulombian Green function with the nonrelativistic parameters X and τ defined in (1.4). Indeed, doing so one omits the relativistic kinematics from the very beginning of the analytical calculation, i.e. some important relativistic kinematics terms in ω^2 , which would in fact exactly cancel some terms due to multipoles, are lost. This is why the spurious kinematics poles occur in the KHW amplitudes for any two-photon process.

In the case of Compton scattering of photons on bound electrons, the nonrelativistic retarded amplitude has even more spurious singularities than Rayleigh amplitude because there are two particles whose energies may change continuously in the final state. The nonrelativistic kinematics gives rise to extra spurious poles and even a spurious cut in the complex plane of the final photon energy ω_2 occurs if $\omega_1 > m/2 + I_B$, as we will show. All these non-physical singularities are displayed by the nonrelativistic retarded amplitude obtained long time ago in the case of Compton scattering from K-shell electrons. Gavrila's results include the contribution of all multipoles but it could be used only in the dipole approximation, its usefulness being severely limited by the spurious singularities influencing the results even at small energies.

The right way to obtain the nonrelativistic amplitudes for a two photon atomic process is to consider the second order S-matrix element involving the sum over the complete set of coulombian Dirac intermediate states $|n\rangle$ of positive and negative energies E_n , and then replace this sum with the coulombian Green function of Dirac equation given by Hostler and Pratt [8], [9]. In this way, one takes into account the relativistic kinematics when performing the integrals involved in the matrix element. Only after performing all the needed integrals, one should consider the nonrelativistic limit of the second order S-matrix elements obtaining the right nonrelativistic amplitudes without any spurious singularity. Thus, the nonrelativistic limit of both the real and imaginary part of Rayleigh amplitudes is correctly obtained.

2 The Second order S-Matrix Element for Two-Photon Processes

There are two Feynman diagrams for the second order amplitudes of a two photon scattering process (fig 1). For sake of simplicity let us consider the ground state of energy $E_0 = \gamma m$ as the initial state of the atomic electron In a relativistic calculation, the matrix element is given by the expression

$$M_{if} = M_{if}(\Omega_1) + M_{if}(\Omega_2), \tag{2.1}$$

where

$$\Omega_1 = \omega_1 + E_0 + i\varepsilon,\ \Omega_2 = -\omega_2 + E_0 + i\varepsilon,\ \gamma = (1 - \alpha^2 Z^2)^{\frac{1}{2}},$$

and

$$M_{if}(\Omega_1) = -m \lim_{\varepsilon \to 0} \underset{\mathrm{n}}{S} \frac{\langle f|e^{-i\,\vec{k}_2\,\vec{r}_2}(\vec{\alpha}\,\vec{s}_2)|n\rangle\ \langle n|\,e^{i\,\vec{k}_1\,\vec{r}_1}(\vec{\alpha}\,\vec{s}_1)|i\rangle}{E_n - (\omega_1 + E_0 + i\varepsilon)}, \tag{2.2}$$

$$M_{if}(\Omega_2) = -m \lim_{\varepsilon \to 0} \underset{\mathrm{n}}{S} \frac{\langle f|e^{i\,\vec{k}_1\,\vec{r}_2}(\vec{\alpha}\,\vec{s}_1)|n\rangle\ \langle n|\,e^{-i\,\vec{k}_2\,\vec{r}_1}(\vec{\alpha}\,\vec{s}_2)|i\rangle}{E_n - (E_0 - \omega_2 - i\varepsilon)}. \tag{2.3}$$

Here, E_1 and E_f are the energies of the K-shell and final electrons, respectively; $\omega_j, \vec{k}_j, \vec{s}_j (j = 1, 2)$ are the energies, momentum and polarization vectors of the incident and final photons respectively, while $|f\rangle$ and $|i\rangle$ denote Dirac spinors for the final and initial states of the electron in the nucleus Coulomb field. The sum over the complete set of intermediate states $|n\rangle$ involves the contributions of both positive and negative frequencies. The energies of the incident and scattered photons are ω_1 and ω_2 respectively. The operator $\vec{\alpha}\,\vec{s}$ is expressed in terms of the three usual 4x4 Dirac matrices. The arbitrary small quantity $\varepsilon > 0$ allows avoiding the singularities when $E_n \approx \omega_1 + E_0$ or $E_n \approx -\omega_2 + E_0$

2.1 Analytic properties of the scattering amplitudes

Inspecting the denominator of the amplitude $M_{if}(\Omega_1)$ we notice that for any positive frequencies we have $E_{n^+} \geq E_0$, thus inelastic resonant Raman scattering occurs for $\omega_1 = E_{n^+} - E_0$ if $E_{n^+} \leq m$, while either the photoeffect or the inelastic Compton scattering occur for $\omega_1 = E_{n^+} - E_0$ if$E_{n^+} \geq m$, when the final electron state belongs to the continuum spectrum. In the complex plane of the energy ω_1 , there are simple poles corresponding to resonant Raman and a cut beginning from the Compton threshold energy $\omega_{th} = m - E_0$. Because the initial electron was considered in the ground state, for the positive frequencies the denominator $E_n - \Omega_2$ of the term $M_{if}(\Omega_2)$ never vanishes. For $E_{n^+} = E_0$ the denominator gets its minimum value ω_2, thus no resonant poles can occur in the term $M_{if}(\Omega_2)$ but the infrared divergence observed by Gavrila [7] is present. For negative frequencies $E_{n^-} \leq -m$ the denominator $E_{n^-} - \Omega_1$ never vanishes and the $M_{if}(\Omega_1)$ amplitude has no singularities. The denominator $E_{n^-} - \Omega_2$ vanishes for any $\omega_2 \geq m + E_0$, thus the term $M(\Omega_2)$ has a cut beginning above the pair-production threshold energy with the created electron in the K-shell $\omega_1 = \omega_{pp} + E_0 = m + 2E_0$.

When the initial state of energy E_i is not the ground state, the amplitude $M_{if}\,(\Omega_1)$ has the analytic properties. For sake of simplicity let's consider the initial electron in the ground state

-For any positive frequencies $E_{n^+} \geq E_i$ so that inelastic resonant Raman scattering occurs for $\omega_1 = E_{n^+} - E_i$ if $E_{n^+} < m$

-If $E_{n^+} \geq m$ the final electron state belongs to the continuum spectrum for $\omega_1 = E_{n^+} - E_i$ either the photoeffect or Compton scattering occurs -For $E_{n^-} \leq -m$ the denominator $E_{n^-} - \Omega_1 < 0$, the term has no poles. Simple poles correspond to resonant Raman, a cut begins from the threshold

About the amplitude $M_{if}\,(\Omega_2)$ we have to keep in mind:

-If $E_{n^+} > E_i$, the denominator gets minimum value so no resonant poles can occur, but an infrared divergence is present when $\omega_2 \to 0$

-For negative frequencies $E_{n^-} \leq m$ the denominator $E_{n^-} - \Omega_2 = 0$ for any $\omega_2 \geq m + E_i$ thus the term $M_{if}\,(\Omega_2)$ has a cut beginning from the pair-production threshold energy $\omega_1 = \omega_{pp} + E_i = m + 2E_i$, with the created electron in the initial state.

In the Figure 2 are displayed physical singularities of the two-photon amplitude.

2.2 Coulombian Green function method

The sum over all intermediate states can be replaced by introducing the Green function of the Dirac equation with Coulombian field $G(\vec{r}_2, \vec{r}_1; \Omega)$

$$G(\vec{r}_2, \vec{r}_1; \Omega) = \underset{\mathrm{n}}{S} \frac{|n\rangle\ \langle n|}{E_n - \Omega} \tag{2.4}$$

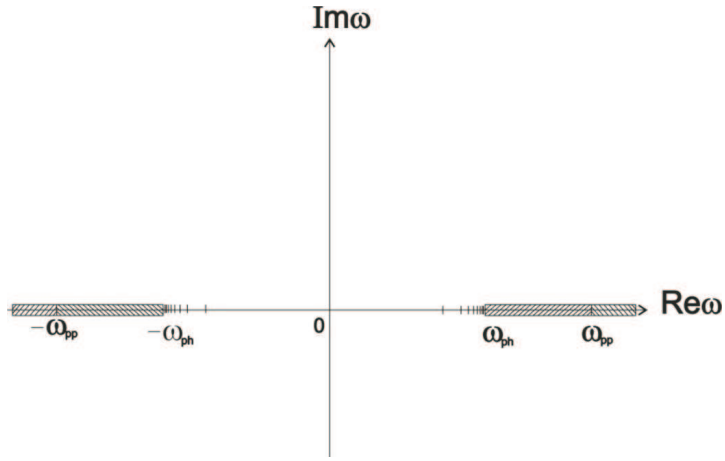

Figure 2: Physical singularities of the amplitudes in the photon energy complex plane

where the sum over all intermediate states $|n\rangle$ is over the complete set of coulombian Dirac spinors i.e. a sum over all positive and negative energies.

$$M_{fi}(\Omega_1) = -m\,\langle f|e^{-i\,\vec{k_2}\,\vec{r_2}}(\vec{\alpha}\,\vec{s}_2)\,G(\vec{r_2},\vec{r_1};\Omega_1)\,e^{i\,\vec{k_1}\,\vec{r_1}}(\vec{\alpha}\,\vec{s}_1)|i\rangle \tag{2.5}$$

$$M_{fi}(\Omega_2) = -m\,\langle f|e^{i\,\vec{k_1}\,\vec{r_2}}(\vec{\alpha}\,\vec{s}_1)\,G(\vec{r_2},\vec{r_1};\Omega_2)\,e^{-i\,\vec{k_2}\,\vec{r_1}}(\vec{\alpha}\,\vec{s}_2)|i\rangle \tag{2.6}$$

where the final state $|f\rangle$ is described by the Dirac spinor $u_f^{(-)}(\vec{r_2})$ belonging to the continuum spectrum with incoming asymptotic spherical waves. The Coulomb Green function for Dirac equation was given by Hostler and Pratt [1963] and Hostler [10]; it can be expressed in the form

$$G(\vec{r_2},\vec{r_1};\Omega) = \frac{1}{2m}\left(i\,\vec{\alpha}\,\nabla_2 - \beta m - \frac{\alpha Z}{r_2} - \Omega\right)\left[I + \frac{1}{2\Omega}\,\vec{\alpha}\left(\vec{P_2} + \vec{P_1}\right)\right] G_0(\vec{r_2},\vec{r_1};\Omega) \tag{2.7}$$

where $G(\vec{r_2},\vec{r_1};\Omega)$ is the Green function of the Schrodinger type equation*:

$$\left(-\frac{1}{2m}\Delta_2 - \frac{\alpha Z\Omega}{m}\frac{1}{r_2} + \frac{m^2-\Omega^2}{2m}\right) G_0(\vec{r_2},\vec{r_1};\Omega) = -\delta(\vec{r_2}-\vec{r_1}) \tag{2.8}$$

or

$$\left(H_0^{Schr} + \frac{X^2}{2m}\right) G_0(\vec{r_2},\vec{r_1};\Omega) = -\delta(\vec{r_2}-\vec{r_1}) \tag{2.9}$$

with

$$X^2 = m^2 - \Omega^2 \;\; and \;\; H_0^{Schr}(\vec{r_2},\Omega) = -\frac{1}{2m}\Delta_2 - \frac{\alpha\,Z\,\Omega}{m}\frac{1}{r_2} \tag{2.10}$$

As Hostler pointed out it follows that the second term in the right parenthesis of eq., representing the first iteration of the "main" term $G_0(\vec{r_2},\vec{r_1};\Omega_1)$, describes the spin contributions to the electronic propagator, while the function $G_0(\vec{r_2},\vec{r_1};\Omega_1)$, itself contains all relativistic kinematics effects via the "changed parameters" $X^2 = m^2 - \Omega^2$ instead the nonrelativistic parameter $X^2_{NR} = -2m\Omega$ and $\frac{\alpha\,Z\Omega}{m}$ instead the nonrelativistic term $\alpha\,Z$).

The first iteration term together with the "main" term $G_0(\vec{r_2},\vec{r_1};\Omega_1)$, represents the Sommerfeld-Maue approximation to the relativistic coulombian Green function. The propagator spin contributions, as given by the first iterative term to the "main" term in a large range of energies. Indeed, in the case of Rayleigh scattering the contribution to the matrix elements $M_{fi}(\Omega)$ of the operator $\frac{\vec{\alpha}\,\vec{P}}{2\Omega}$ are small

either for photon energies up to several times the photoeffect threshold, where the full nonrelativistic approach gives excellent predictions, or for large photon energies as was already proved. Taking into account that

$$\left(u_f^{(-)}(\vec{r_2})\right)^+ \left(\vec{\alpha}\,\vec{P} + \beta m - \frac{\alpha Z}{r_2} - E_f\right) = 0,$$

we get

$$M_{fi}\left(\Omega_1\right) = -\frac{1}{2}\int d^3r_1 \int d^3r_2 u_f^+\left(\vec{r}_2\right)\left\{\left[\vec{\alpha}\vec{s}_2\left(\Omega_1 - E_f\right) + \vec{s}_2\vec{P}_2\right] e^{i\left(\vec{k}_1\vec{r}_1 - \vec{k}_2\vec{r}_2\right)}\right\} \tag{2.11}$$

$$\left[I - \frac{1}{2\Omega_1}\vec{\alpha}\left(\vec{P_1} + \vec{P_2}\right)\right] G_0(\vec{r_2}, \vec{r_1}; \Omega_1)\Bigg\}\, \vec{\alpha}\,\vec{s_1}\, u_i(\vec{r_1})$$

The above expression may be written in the momentum space as

$$M_{fi}\left(\Omega_1\right) = -\frac{1}{2}\int d^3p_1 \int d^3p_2 u_f^+\left(\vec{r}_2\right)\left\{\left[\vec{\alpha}\vec{s}_2\left(\Omega_1 - E_f\right) + \vec{s}_2\vec{P}_2\right] e^{i\left(\vec{k}_1\vec{r}_1 - \vec{k}_2\vec{r}_2\right)}\right\} \tag{2.12}$$

$$\times \left[I + \frac{1}{2\Omega_1}\vec{\alpha}\left(\vec{p_1} - \vec{p_2}\right)\right] G_0(\vec{p_2}, \vec{p_1}; \Omega_1)\Bigg\}\left(\vec{\alpha}\,\vec{s_1}\right) u_i(\vec{r_1})$$

and a similar expression for $M_{fi}(\Omega_2)$ with $\vec{k}_2 \leftrightarrow -\vec{k}_1$. The Coulombian Green function in momentum space is given by integral representation due to Schwinger [9],

$$G_0(\vec{p_2}\,\vec{p_1}; \Omega) = -\frac{mX^3}{2\pi^2}\left(\frac{ie^{i\pi\tau}}{2\sin\pi\tau}\right)\int_1^{(0+)} \rho^{-\tau}\frac{d}{d\rho} \tag{2.13}$$

$$\left(\frac{1-\rho^2}{\rho}\frac{1}{\left[X^2\left(\vec{p_1} - \vec{p_2}\right)^2 + \left(p_1^2 + X^2\right)\left(p_2^2 + X^2\right)(1-\rho)^2/4\rho\right]^2}\right) d\rho$$

with

$$\tau = \frac{\alpha Z\Omega}{X},\ X^2 = m^2 - \Omega^2$$

For any two photon atomic process the amplitudes involve a basic sixfold integral which was calculated long time ago in connection with the elastic scattering of photons by the K-shell electrons. The expression may be written in terms of the integral because the integral representation for the Coulomb-Green function in momentum space $G_0(\vec{p_2}\,\vec{p_1}; \Omega)$, the integral representation for the final electron wave function in momentum space $u_f(\vec{p})$ and the initial bound electron wave function $u_i(\vec{p})$ lead to such a term. Indeed, the expressions we need for the amplitudes are obtained by Gavrila and Costescu [10,11]

$$\frac{d}{d\rho}\left[\left(\frac{1-\rho^2}{\rho}\right) J\left(X^2; \lambda, \mu\right)\right] = \frac{16\pi^4}{X^2}\frac{1}{c(\Omega, \rho)} \tag{2.14}$$

where

$$c(\Omega, \rho) = \left[(X+\lambda)^2 + k_1^2\right]\ \left[(X+\mu)^2 + \kappa_2^2\right]\ \left[1 - 2\rho\, s(\Omega, \mu, \vec{\kappa_2}) + \rho^2 p(\Omega, \mu, \vec{\kappa_2})\right] \tag{2.15}$$

with

$$s(\Omega, \mu, \vec{\kappa_2}) = \frac{\left(\lambda^2 + k_1^2 - X^2\right)\left(\mu^2 + \kappa_2^2 - X^2\right) + 4\left(\vec{k_1}\,\vec{\kappa_2}\right)X^2}{\left[(X+\lambda)^2 + k_1^2\right]\ \left[(X+\mu)^2 + \kappa_2^2\right]},$$

$$p(\Omega,\mu,\vec{\kappa_2})=\frac{\left[(X-\lambda)^2+k_1^2\right]\left[(X-\mu)^2+\kappa_2^2\right]}{\left[(X+\lambda)^2+k_1^2\right]\left[(X+\mu)^2+\kappa_2^2\right]},$$

Finally, all needed integrals over the variable ρ are of the kind

$$\frac{ie^{-i\pi a}}{2\sin\pi a}\int\limits_1^{(0+)}\frac{\rho^{a-1}}{(1-\rho\,s+\rho^2p)^{b_1}\,(1-\rho\,s'+\rho^2p')^{b3}}d\rho$$

with

$$a=n_0-\tau,b_1=n_1-\nu,b_3=n_3+\nu$$

where n_0,n_1,n_3 some specific natural numbers, and $\nu=\alpha Z\Omega/ip$ if the final state belongs to continuum spectrum (Compton scattering, two photon ionization). In the simpler case of a bound-bound transition, $\nu=0$ and $b_3=0$.

The coefficients

$$s(\Omega_1)=x(\Omega_1)+y(\Omega_1),s(\Omega_2)=x(\Omega_2)+y(\Omega_2),s'(\Omega_1)=x'(\Omega_1)+y'(\Omega_1),s'(\Omega_2)=x'(\Omega_2)+y'(\Omega_2),$$

$$p(\Omega_1)=x(\Omega_1)y(\Omega_1),p(\Omega_2)=x(\Omega_2)y(\Omega_2),p'(\Omega_1)=x(\Omega_1)y(\Omega_1),p'(\Omega_2)=x(\Omega_2)y(\Omega_2),$$

are cumbersome but known functions of the photon energy and scattering angle such integrals may be performed observing that they are similar to the integral representation of the Lauricella functions

$$F_D\left(a;b_1,b_2,b_3,b_4;c;x,y,x',y'\right) \tag{2.16}$$

$$=-\frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)}\left(\frac{ie^{-i\pi a}}{2\sin\pi a}\right)\int\limits_1^{(0+)}\frac{\rho^{a-1}(1-\rho)^{c-a-1}}{(1-\rho\,x)^{b_1}\,(1-\rho\,y)^{b_2}\,(1-\rho\,x')^{b_3}\,(1-\rho\,y')^{b_4}}d\rho$$

Inspecting the above integral representation and the integrals we observe that each of them introduces a Lauricella function with $c=a+1$, $b_1=b_2$, are cumbersome but known functions of the photon energy and scattering angle where c and a are the last and the first parameters respectively:

$$\frac{ie^{-i\pi a}}{2\sin\pi a}\int\limits_1^{(0+)}\frac{\rho^{a-1}}{(1-\rho\,s+\rho^2p)^{b_1}\,(1-\rho\,s'+\rho^2p')^{b3}}d\rho \tag{2.17}$$

$$=\frac{ie^{-i\pi a}}{2\sin\pi\,a}\int\limits_1^{(0+)}\frac{\rho^{a-1}}{(1-\rho\,x)^{b_1}\,(1-\rho\,y)^{b1}\,(1-\rho\,x')^{b_3}\,(1-\rho\,y')^{b_3}}d\rho$$

Fortunately, the integrals that we meet have no cut between 0 and 1 so that the integral representation of Lauricella functions becomes significantly simpler:

$$\frac{1}{a}F_D[a;b_1,b_1,b_3,b_3;a+1;x(\Omega_j),y(\Omega_j),x'(\Omega_j),y'(\Omega_j)] \tag{2.18}$$

$$=\int\limits_0^1\frac{\rho^{a-1}}{(1-\rho\,x)^{b_1}\,(1-\rho\,y)^{b1}\,(1-\rho\,x')^{b_3}\,(1-\rho\,y')^{b_3}}d\rho$$

The above mentioned particularities $c=a+1,b_1=b_2,b_3=b_4$ allows us to write all invariant amplitudes with the minimum number of distinct Lauricella functions F_D and to perform a fast and accurate numerical calculation.

In the case of a bound-bound two photon transition, the amplitudes are expressed in terms of Appell functions F_1

$$F_1\left(a,b_1,b_2;c;x,y\right)=\frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)}\left(\frac{ie^{-i\pi a}}{2\sin\pi a}\right)\int\limits_1^{(0+)}\frac{\rho^{a-1}(1-\rho)^{c-a-1}}{(1-\rho\,x)^{b_1}\,(1-\rho\,y)^{b_2}}d\rho$$

Again we observe that $c = a + 1$, $b_2 = b_1$ so that the integral representation of Appell functions becomes simpler

$$\frac{1}{a} F_1 \left(a, b_1, b_1; a+1; x, y\right) = \int\limits_0^1 \frac{\rho^{a-1}}{\left(1-\rho\, x\right)^{b_1} \left(1-\rho\, y\right)^{b1}} d\rho \tag{2.19}$$

For this particular values of the parameters, there are some useful recursion relationships which allow to express the cross-section with only a few Lauricella functions in the case of Compton scattering and Appel functions in the case of bound-bound tranzitions

The forward scattering amplitude of the elastic scattering gives via the optical theorem the total cross-section for both atomic photo effect and pair production (with the final electron in K-shell):

$$\sigma_{ph} = \frac{4\pi m}{\alpha\omega} r_0^2 \left|\mathrm{Im} M\left(\Omega_1, \omega, \theta\right) = 0\right|;$$

$$\sigma_{pp} = \frac{4\pi m}{\alpha\omega} r_0^2 \left|\mathrm{Im} M\left(\Omega_2, \omega, \theta\right) = 0\right|;$$

In the following we give the nonrelativistic limit of the Compton and Rayleigh scattering amplitudes in the case of K-shell electrons as well as for atomic photoeffect (Costescu, Spanulescu, Stoica, [6] and [12].

3 The Nonrelativistic Limit of the Two Photon Amplitude

The two-photon amplitude may be also written

$$M_{fi} = s_{1j} s_{2k} \left[\Pi_{jk} + \Pi_{jk}\left(\Omega_1\right) + \Pi_{jk}\left(\Omega_2\right)\right], \tag{3.1}$$

where we have dropped out the first iterative term containing spin terms, thus we do not consider spin corrections to the electron propagator. Also, it is obvious that this approach is valid in the nonrelativistic limit $\omega_1 \sim \alpha^2 Z^2 m << m$ where there is no iterative term.

Taking into account that

$$\begin{aligned}\left(\Omega - E_f\right) G_0(\vec{r_2}\,\vec{r_1}; \Omega) &= \underset{\mathrm{n}^+}{S} \left(-1 + \frac{E_{n^+} - E_f}{E_{n^+} - \Omega}\right) \left|n^+\right\rangle \left\langle n^+\right| \\ &= -\delta\left(\vec{r_2} - \vec{r_1}\right) + \left(H_0(\vec{r_2}) - E_f\right) G_0(\vec{r_2}\,\vec{r_1}; \Omega)\end{aligned} \tag{3.2}$$

and

$$\left(\vec{\alpha}\,\vec{s_2}\right)\left(\vec{\alpha}\,\vec{s_1}\right) + \left(\vec{\alpha}\,\vec{s_1}\right)\left(\vec{\alpha}\,\vec{s_2}\right) = 2\left(\vec{s_2}\,\vec{s_1}\right) \cdot I$$

we get

$$s_{1j} s_{2k} \vartheta_{jk} \cong \vartheta\, \vec{s_1}\,\vec{s_2} + s_{1j} s_{2k} \vartheta_{jk}$$

where

$$\vartheta = \int\limits_{R^3} d^3 r \left(u_f^{(-)}(\vec{r_2})\right)^+ e^{i(\vec{k_2} - \vec{k_1})\,\vec{r}}\, u_i(\vec{r}) = \left\langle f\right| e^{i(\vec{k_2} - \vec{k_1})\,\vec{r}} \left|i\right\rangle$$

is the relativistic form factor.

Long time ago Hostler proved that it is possible to obtain the relativistic Coulomb continuum states a limiting case of the physical Green's function for Dirac equation both for positive and negative frequency states and both for incoming and outgoing wave boundary conditions. According to the Hostler result, in our case, to the iterated Green function

$$\left[I + \frac{1}{2\Omega}\,\vec{\alpha}\left(\vec{P_2} + \vec{P_1}\right)\right] G_0(\vec{r_2}\,\vec{r_1}; \Omega)$$

corresponds the iterated Dirac wavespinor with asymptotic behavior given by a spherical incoming wave

$$u^{(-)}_{\vec{p}\,\mu}(\vec{r}) = \left(I + \frac{\vec{\alpha}\,\vec{P_2}}{2E_f} \right) u^{(-)}_{\vec{p}}(\vec{r}) u_\mu(\vec{p})$$

where

$$u^{(-)}_{\vec{p}}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \Gamma\left(1 + i\,|\nu|\right) e^{\frac{\pi|\nu|}{2}} e^{i\,\vec{p}\,\vec{r}}\, {}_1F_1\left(-i\,|\nu|\,,\ 1;\ -i\left(\vec{p}\,\vec{r} + p\,r\right)\right) \tag{3.3}$$

and $u_\mu(\vec{p})\underline{\mu}c12$ is a normalized Dirac spinor describing a free electron with momentum $\vec{p}$ and polarization μ. The momentum p and the parameter are given by relativistic kinematics

$$p = \sqrt{E_f^2 - m^2}, \quad \nu = \frac{\alpha\, Z E_f}{i p} \tag{3.4}$$

and

$$E_f = m + \omega_{2\,\max} - \omega_2$$

where

$$\omega_{2\,\max} = \omega_1 - I_B = \omega_1 - (1-\gamma)m \tag{3.5}$$

The dominant term $u^{(-)}_{\vec{p}}(\vec{r})$ of the spinor $u^{(-)}_{\vec{p}\,\mu}(\vec{r})$ is the solution of the Schrdinger type equation

$$\left(-\frac{1}{2m}\Delta - \frac{\alpha Z}{r} - E_f \right) u^{(-)}_{\vec{p}}(\vec{r}) = 0 \tag{3.6}$$

For any incoming photon energy ω_1, in the hard photon region of Compton spectrum there is an energy range where we may consider that the final electron moves nonrelativistically, so we should neglect the spin term of the spinor. In accordance with dropping out the Sommerfeld-Maue spin corrections to the propagator, we may expect that this approach may be considerd valid for the most part of the Compton spectrum. For nonrelativistic energy values of the incident photon $\omega_1 << m$, this is right for the whole Compton spectrum.

We observe that $\left(H_0^{Schr}(\vec{r_2}, \Omega) - E_f \right) u^{(-)}_{\vec{p}}(\vec{r_2}) = 0$ if $\omega_1 \leq \alpha\, Z\, m$ so that the term ϑ_{jk} in equation vanishes. Indeed, if $\omega_1 \leq \alpha\, Z\, m$ both for $\Omega_1 = \gamma\, m + \omega_1$ and $\Omega_2 = \gamma\, m - \omega_2$ we may put $\frac{\alpha\, Z\, \Omega}{m\, r} \cong \frac{\alpha\, Z}{r}$, because the neglected term $\frac{\alpha^2\, Z^2}{r}$ is in the same $\alpha\, Z$ order as the terms which are involved in the second iteration to the main term of the Green function and have already been neglected. The equation becomes

$$s_{1j} s_{2k} \vartheta_{jk} = \vec{s_1}\,\vec{s_2}\,\vartheta$$

where the final state in ϑ is a Schrdinger type eigenfunction, involving relativistic kinematics. In order to calculate the matrix element ϑ, we have to observe that the K-shell Dirac spinor $u_i(\vec{r_1})$ contains the "negative power" factor $\left(\frac{Z\,r}{a_0}\right)^{\gamma-1}$ which gives rise to strong relativistic effects in the case of large momentum transfers and high Z targets, when small r distances have a major contribution to the matrix element of the process. These effects are increasing as the energy ω_1 increases. However, if $\omega_1 < \alpha Z m$ we may consider that the photon momentum transfer $\vec{\Delta} = \vec{k_1} - \vec{k_2}$ is small for any scattering angle θ, so that the matrix element value is given mainly by the r values close to the ion Bohr radius $\frac{a_0}{Z}$ and

$$\left(\frac{Z\,r}{a_0}\right)^{\gamma-1} = 1 + (1-\gamma)\ln\left(\frac{a_0}{Z}\frac{1}{r}\right) + ... \cong 1$$

In the next figures we compare our numerical results predicted by our formulae with the full relativistic numerical calculations of Bergstrom, Suric, Pisk and Pratt [1993]. We compare the Compton doubly differential cross-section

$$\frac{d^2\sigma}{d\Omega_k 2 d\omega_2} = \frac{1}{2}\int\limits_{\Omega_p} \sum_{\vec{s_1},\vec{s_2}} |M|^2 d\Omega \frac{\omega_2}{\omega_1} r_0^2 \tag{3.7}$$

and also the singly differential cross-section which gives the Compton angular distribution

$$\frac{d\sigma_B}{d\Omega_k 2} = \frac{r_0^2}{2}\int\limits_{\Omega_p} \int\limits_{\omega_{thr}}^{\omega_{2\,\max}} \sum_{\vec{s_1},\vec{s_2}} |M|^2 d\Omega \; d\omega_2 \tag{3.8}$$

We also calculated the ratio $d\sigma_B/d\sigma_{free}$ between the singly differential cross section for a K-shell bound electron, and the free electron singly differential cross-section given by the well known Klein-Nishina formula [1929].

For numerically evaluating the cross-sections, the most time-expensive part is the calculation of the Lauricella functions of D type, depending of six parameters and four variables, all complex, involved in the expressions of the amplitudes. Among the various methods eligible for computing the higher order transcendental functions, we tested two: series expansion and integral representation. The second method proved to be more efficient and therefore we consistently used it in all our calculations. Although the general integral representation of these functions may demand a large quantity of calculus, by appropriate using their actual characteristics, the computing speed can be greatly improved. Thus, taking into account the normal integral representation of Lauricella D type function, one can write these functions in the form:

$$\frac{1}{a}F_D\left(a;b_1,b_1,b_2,b_2;a+1;x,y,x',y'\right) = \int\limits_0^1 \frac{\rho^{a-1}}{\left(1-\rho\, s(\Omega_j)+\rho^2\, p(\Omega_j)\right)^{b_1}\left(1-\rho\, s'(\Omega_j)+\rho^2\, p'(\Omega_j)\right)^{b_2}} d\rho \tag{3.9}$$

Analogue, Appell functions are computed making use of the simple integral representation

$$\frac{1}{a}F_1\left(a;b,b,a+1;x,y\right) = \int\limits_0^1 \rho^{a-1}\frac{1}{\left(1-\rho s\left(\Omega\right)+\rho^2 p\left(\Omega\right)\right)^b} d\rho \tag{3.10}$$

which allow us to get the angular distribution of Rayleigh scattering.

4 Numerical Results and Conclusions

In the figures [3-5] we present the angular distribution predictions for Compton scattering by a K-shell electron of the elements with Z=30, Z=50 and Z=79 which are all in good agreement with relativistic numerical computations. We mention that comparing the predictions given by our nonrelativistic limit for Compton scattering with relativistic numerical calculations performed with Cray supercomputers by Bergstrom et al. (13) a good accuracy within 5 percent for photon energies up to 200 KeV. The nonrelativistic limit gives with high accuracy the profile of Compton pick. It allows to obtain with accuracy the momentum distribution of K-shell electrons even in the case of high Z atoms. Comparing the predictions given by the nonrelativistic limit of the amplitude in the case of Rayleigh scattering by the K-shell electrons with relativistic numerical results obtained by Kissel et al. [14]. The same good concordance within 5 percent is found. An excellent agreement is also found in the case of K-shell photo-effect comparing with relativistic numerical data obtained by Scofield [15] and Kissel et al. [14]. This concordance between the nonrelativistic limit and full numerical relativistic predictions shows that spin effects are small for unexpectedly large energies. Also it is proven analiticaly and numericaly that important cancelations occur between quadratic retardation and relativistic kinematics terms. In a large range of not too high energies the linear terms in the photon energy due to retardation represent the main correction to the dipole nonrelativistic result leading to excelent predictions.

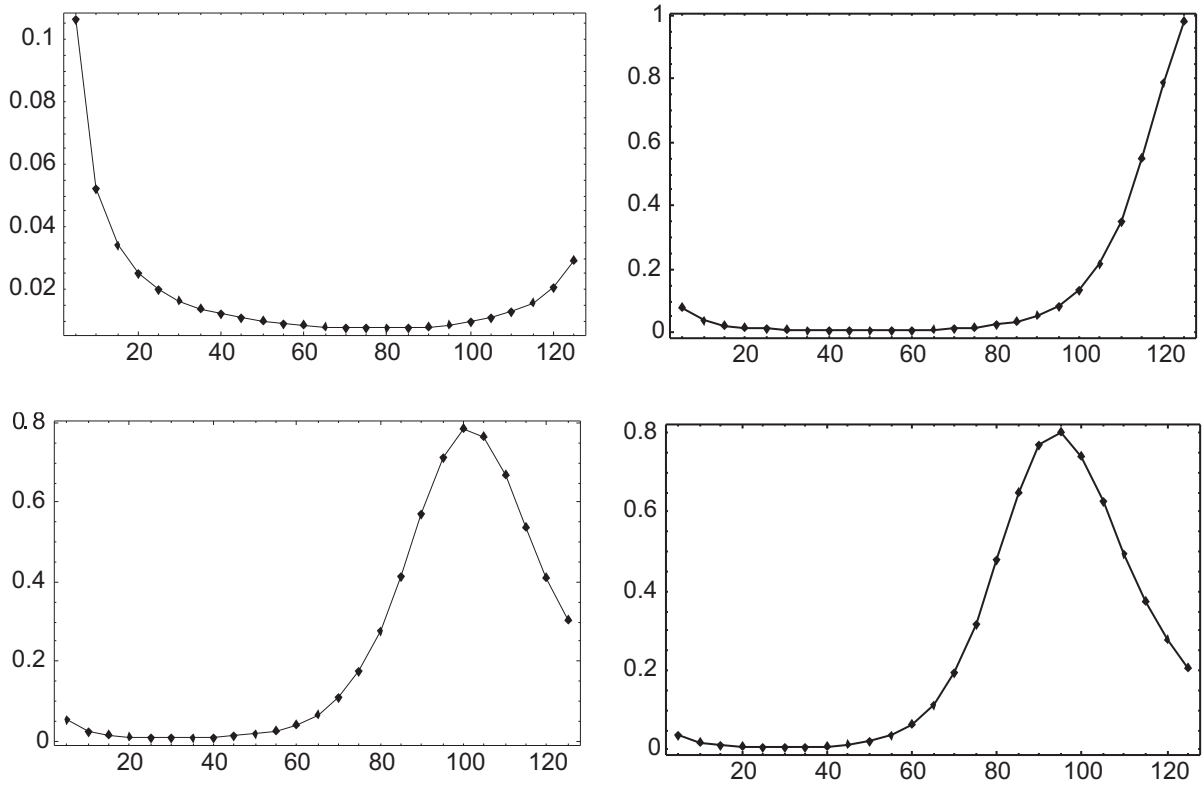

Figure 3: Doubly differential cross sections for the scattering of 145 KeV ohitins from a K-shell electron of Zn (Z=30), for scattering angles $\theta = 0; \pi/3; 2\pi/3; \pi$

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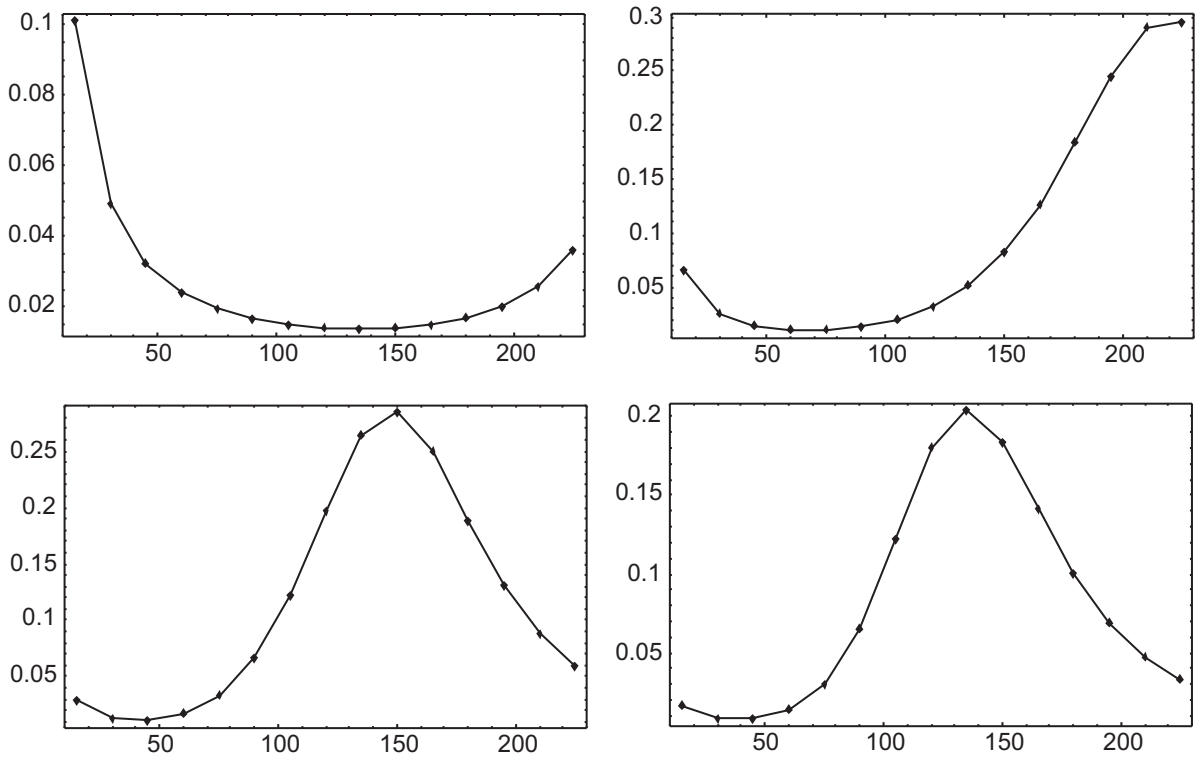

Figure 4: Doubly differential cross sections for the scattering of 145 KeV ohitins from a K-shell electron of Sn (Z=50), for scattering angles $\theta = 0; \pi/3; 2\pi/3; \pi$

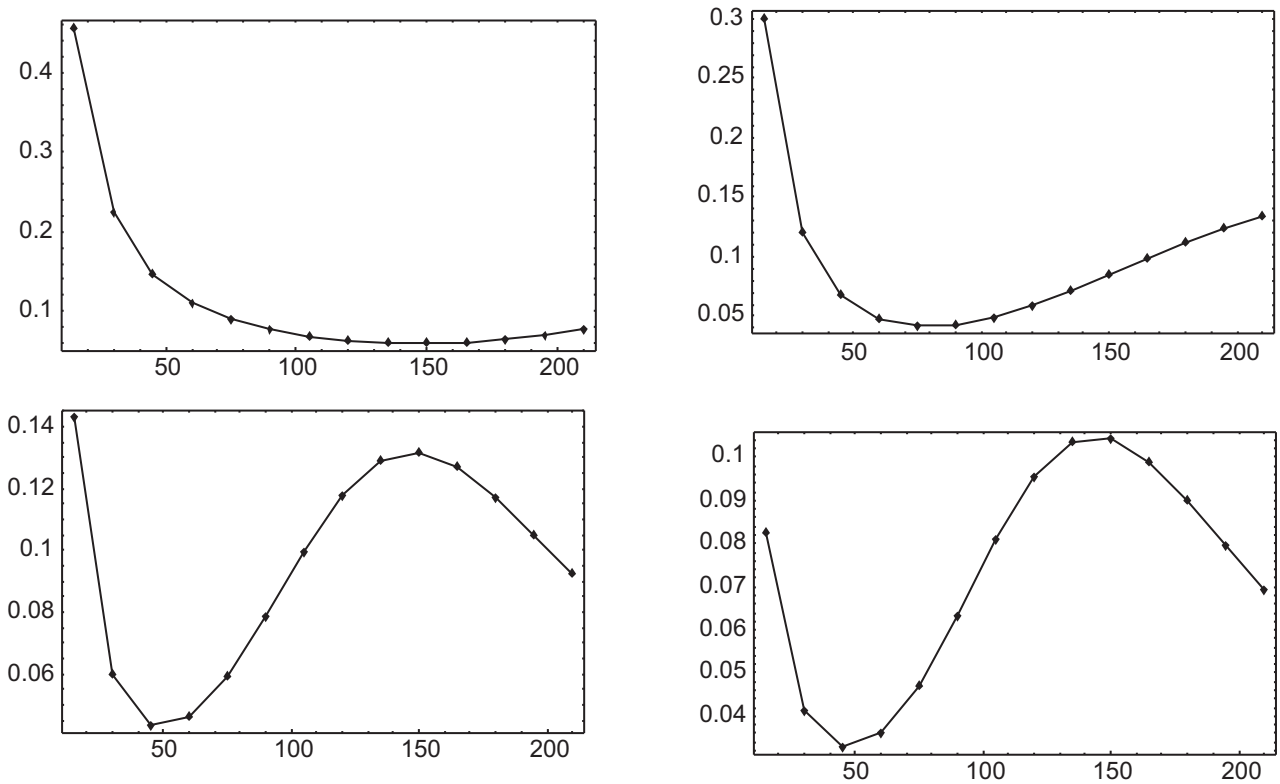

Figure 5: Doubly differential cross sections for the scattering of 145 KeV ohitins from a K-shell electron of Au (Z=79), for scattering angles $\theta = 0; \pi/3; 2\pi/3; \pi$

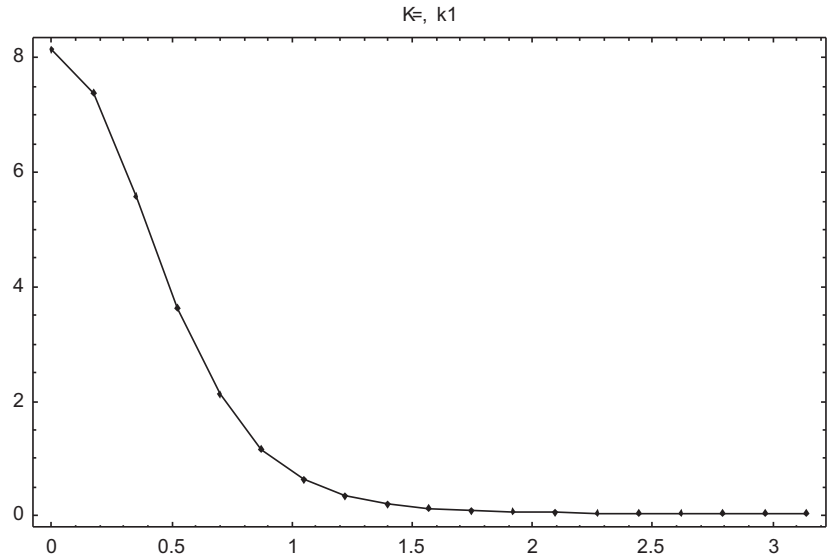

Figure 6: Angular distribution of the Rayleigh scattering for a K-Shell electron of Sn(Z=50) at 320 KeV

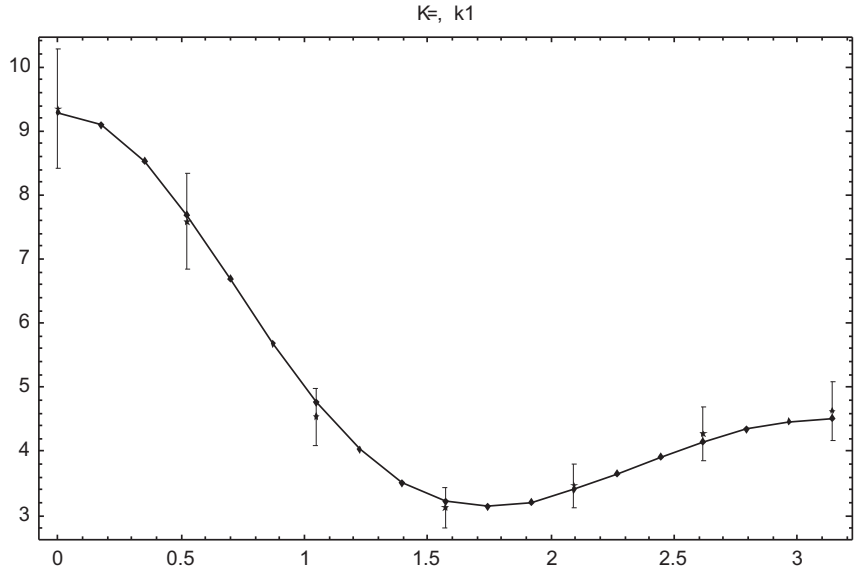

Figure 7: Angular distribution of the Rayleigh scattering for a K-Shell electron of Pb(Z=82) at 158 KeV

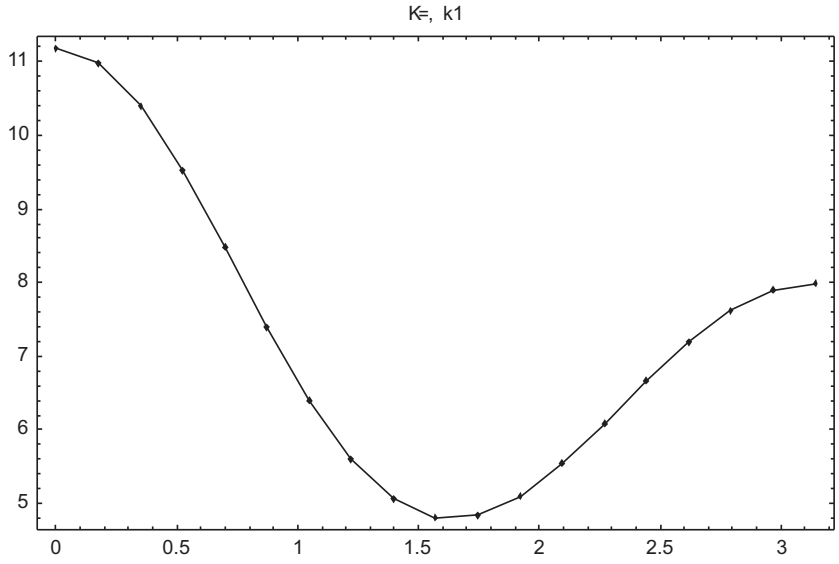

Figure 8: Angular distribution of the Rayleigh scattering for a K-Shell electron of U(Z=92) at 145 KeV

References

[1] H.A. Kramers and W. Heisenberg, Z. Physik 31, 681 (1925);

[2] I. Waller, Z. Phys. 58, 75 (1928);

[3] A. Costescu, P.M. Bergstrom, C. Dinu, R.H. Pratt, Phys. Rev. A 50, 1390(1994);

[4] P.M. Bergstrom, Lynn Kissel, R.H. Pratt and A. Costescu, Acta Cryst. A53, 7(1997);

[5] J. Fisher, Ann. Phys. (Leipzig) 8, 821(1931); 11, 489(1931);

[6] A. Costescu ans S. Spanulescu, Phys. Rev. A 73, 022702(2006);

[7] L. Hostler, R.H. Pratt, Phys. Rev. Let. 10, 469(1963);

[8] A. Costescu, S. Spanulescu, Phys. Rev. A **73**, 022702 (2006);

[9] J. Schwinger, J. Math. Phys., 5, 1606(1964);

[10] M. Gavrila and A. Costescu, Phys. Let. 28 A, 614(1969);

[11] M. Gavrila and A. Costescu, Phys. Rev. A, 2, 1752(1970);

[12] A. Costescu, S. Spanulescu and C. Stoica, J. Phys. B:At. Mol. Opt. Phys. 40(2007)2995;

[13] P.M. Bergstrom, T. Suric, K. Pisk, and R.H. Pratt, Phys. Rev. A 48, 1134 (1993);

[14] Kissel L, Pratt R.H. and Roy S. C 1980 Phys. Rev. A 22 (1970);

[15] Scofield J H 1973 Lawrence Radiation Laboratory Report No. CRL 51326, Livermore, CA;