Analytical properties and numerical calculations of high transcendental functions involved in the relativistic amplitudes of two photon atomic processes

ADRIAN COSTESCU
Department of Theoretical Physics and Mathematics
University of Bucharest
Atomistilor 5, Bucharest Magurele
ROMANIA

SEVER SPANULESCU
Department of Physics
Hyperion University of Bucharest,
Calea Calarasilor nr. 169, Bucharest
ROMANIA

CRISTIAN STOICA
Department of Theoretical Physics and Mathematics
University of Bucharest
Atomistilor 5, Bucharest Magurele
ROMANIA

Abstract: - The high transcendental functions that occur in the relativistic expressions of the amplitudes of the two photon atomic processes are analytically treated taking advantage of their specific parameters values. We present some identities and recurrence relationships that allow reducing the number of needed Appell functions and transform their imaginary part in terms of Gauss hypergeometric functions. If the physical model takes into account only the terms up till the fourth power in αZ in the real part and the seventh power in the imaginary part, some transcendental functions may be reduced to elementary functions. The numerical results obtained using the presented methods were compared with other's authors results, displaying a very good agreement.

Key-Words: - Appell functions, Gauss hypergeometric functions, relativistic atomic processes

1 Introduction

It is known that high transcendental functions as Lauricella F_D Appell F_1 and Gauss hypergeometric functions ${}_2F_1$ systematically arise in the expressions of the scattering amplitudes of both inelastic and elastic two photon atomic processes. Moreover, the imaginary part of the elastic forward scattering amplitude gives (via the optical theorem) the cross sections of photoeffect and pair-production with the electron created in a bound state, so that a good knowledge of analytical properties of the Appell functions allows to get simple expressions for these one photon processes.

Some time ago it was proved that in any two photon atomic process some important retardation and relativistic kinematics terms are alike and cancel each other [1],[2]. That extended the validity of the nonrelativistic limit for Compton, Rayleigh and photoeffect K-shell cross sections up to unexpected large photon energies for the whole spectrum.

For energies above 400 keV spin effects become important and spin terms must be considered in order to obtain accurate results. The bound electron states must be described with Dirac spinors. The expressions of the amplitudes become very computing demanding and a large number of higher transcendental functions have to be handled [3],[4].

In this paper we show that in the case of elastic scattering in a full relativistic approach the same high transcendental Appell functions as in the nonrelativistic approximation but their parameters obey relativistic kinematics. This implies obtaining new analytical recursion relations for the Appell's functions involved in the amplitude expressions. That allows to keep the minimum number of distinct Appell's functions.

2 Brief presentation of the transition amplitudes for two photon elastic processes

The Rayleigh amplitude is given by the sum of the contributions of two Feynmann diagrams:

$$\mathfrak{M}_{\mu1\mu2} = \mathfrak{M}_{\mu1\mu2}(\Omega_1) + \mathfrak{M}_{\mu1\mu2}(\Omega_2) \qquad (1)$$

where

$$\mathfrak{M}_{\mu1\mu2}(\Omega_1) = -m\iint_{R^3} d^3r_1 d^3r_2 u^+_{\mu_2}(\vec{r}_2)(\vec{\alpha}\cdot\vec{s}_2)e^{-i\vec{k}_2\cdot\vec{r}_2}$$
$$\times G(\vec{r}_2,\vec{r}_1;\Omega_1)e^{i\vec{k}_1\cdot\vec{r}_1}(\vec{\alpha}\cdot\vec{s}_1)u_{\mu_1}(\vec{r}_1) \qquad (2)$$

$$\mathfrak{M}_{\mu1\mu2}(\Omega_2) = -m\iint_{R^3} d^3r_1 d^3r_2 u^+_{\mu_2}(\vec{r}_2)(\vec{\alpha}\cdot\vec{s}_1)e^{i\vec{k}_1\cdot\vec{r}_2}$$
$$\times G(\vec{r}_2,\vec{r}_1;\Omega_2)e^{-i\vec{k}_2\cdot\vec{r}_1}(\vec{\alpha}\cdot\vec{s}_2)u_{\mu_1}(\vec{r}_1) \qquad (3)$$

In the eqs. (2) and (3) the incoming photon has the energy ω, momentum $\vec{k}_1$ and polarization vector $\vec{s}_1$ while the outgoing photon has the momentum $\vec{k}_2$ and polarization vector $\vec{s}_2$ while $G(\vec{r}_2,\vec{r}_1;\Omega)$ is the relativistic coulomb Green function given by Hostler [4] and Hostler and Pratt [5]

$$G(\vec{r}_2,\vec{r}_1;\Omega)=\sum_n \frac{u_n(\vec{r}_2)u_n^+(\vec{r}_1)}{E_n-\Omega}$$
$$=-\left(\vec{\alpha}\cdot\vec{P}_2+\beta m+\frac{\alpha Z}{r_2}+\Omega\right)G_I(\vec{r}_2,\vec{r}_1;\Omega) \tag{4}$$

with α the Sommerfeld constant, $\vec{\alpha}$ and β Dirac matrices, Z the atomic number, $E_0=\gamma m$, $\gamma=\left(1-\alpha^2Z^2\right)^{1/2}$ the ground state energy, $\Omega_1=E_0+\omega+i\varepsilon$, $\Omega_2=E_0-\omega-i\varepsilon$ and

$$G(\vec{r}_2,\vec{r}_1;\Omega)\approx\left[1-\frac{1}{2\Omega}\vec{\alpha}\cdot\left(\vec{P}_1+\vec{P}_2\right)\right.$$
$$\left.+\frac{1}{8\Omega^2}\left(\vec{P}_1+\vec{P}_2\right)^2\right]G_0(\vec{r}_2,\vec{r}_1;\Omega)+\pi\frac{\alpha Z}{\Omega} \tag{5}$$
$$\times G_0(\vec{r}_2,0;\Omega)G_0(0,\vec{r}_1;\Omega)$$

where the first two terms are due to Hostler [5] and the other two representing the second iteration are given by us.

The main term $G_0(\vec{r}_2,\vec{r}_1;\Omega)$ is the solution of a Schrődinger-type equation

$$\left(\Delta_2+\frac{2\tau X}{r_2}-X^2\right)G_0(\vec{r}_2,\vec{r}_1;\Omega)=\delta(\vec{r}_2-\vec{r}_1) \tag{6}$$

with the parameters

$$X=\sqrt{m^2-\Omega^2}\ ,\ \operatorname{Re}X>0\,;\ \tau=\frac{\alpha Z\Omega}{X} \tag{7}$$

and $X=-i|X|$ above the threshold. The parameters X and τ given by eq. (7) obey relativistic kinematics.

We want to point out that the particular Green function $G_0(\vec{r},0;\Omega)$ due to Martin and Glauber [6] has a simple and extremely useful form,

$$G_0(\vec{r},0;\Omega)=-\frac{1}{4\pi r}\Gamma(1-\tau)W_{\tau,1/2}(2Xr) \tag{8}$$

where $W_{\tau,1/2}(2Xr)$ is the Whittaker function.

In order to evaluate the scattering amplitudes we write the ground state Dirac spinor putting in evidence the "rest frame" spinor χ_μ in momentum representation [7]:

$$u_\mu(\vec{p})=\mathfrak{N}\left[a(p)+\frac{1}{2}\frac{(\vec{\alpha}\cdot\vec{p})}{m}b(p)\right]\chi_\mu=u(\vec{p})\chi_\mu$$

$$a(p)=(1-\gamma)\lambda_0\int_0^\infty dx\,x^{-\gamma}\frac{1+x}{\left[p^2+\lambda_0^2(1+x)^2\right]^2}$$

$$b(p)=2\frac{1-\gamma}{1+\gamma}\lambda_0\int_0^\infty dx\,x^{-\gamma}\frac{1}{\left[p^2+\lambda_0^2(1+x)^2\right]^2}$$

$$\mathfrak{N}=\left[\frac{2^{2\gamma+1}\lambda_0^3}{\pi^2}\frac{1+\gamma}{\Gamma(2\gamma+1)}\right]^{\frac{1}{2}}\frac{1}{\Gamma(2-\gamma)}$$

$$\chi_\mu^+=\begin{cases}(1,0,0,0)\ if\ \mu=1/2\\(0,1,0,0)\ if\ \mu=-1/2\end{cases}$$

as well as in coordinate representation:

$$u_\mu(\vec{r})=\left(1+i\frac{aZ}{1+\gamma}\frac{\vec{\alpha}\vec{r}}{r}\right)a(r)\chi_\mu,$$
$$a(r)=\left[\frac{\lambda_0^3}{\pi}\frac{1+\gamma}{\Gamma(2\gamma+1)}\right]^{1/2}(2\lambda_0 r)^{\gamma-1}e^{-\lambda_0 r},$$
$$\lambda_0=\alpha Zm \tag{9}$$

Taking into account that $u_\mu^+(\vec{r}_2)$ is a Dirac spinor, from eqs. (2), (4) and (5) we get

$$\mathfrak{M}_{\mu_1\mu_2}(\Omega_1)=\mathfrak{M}_{\mu_1\mu_2}^{mom}(\Omega_1)+\mathfrak{M}_{\mu_1\mu_2}^{coor}(\Omega_1) \tag{10}$$

where

$$\mathfrak{M}_{\mu_1\mu_2}^{mom}(\Omega_1)=m\iint_{R^3}d^3p_1d^3p_2u_{\mu_2}^+\left(\vec{p}_2-\vec{k}_2\right)$$
$$\times\left[\omega(\vec{\alpha}\cdot\vec{s}_2)+(\vec{\alpha}\cdot\vec{s}_2)\left(\vec{\alpha}\cdot\vec{k}_2\right)+2(\vec{s}_2\cdot\vec{p}_2)\right]$$
$$\times\left[1-\frac{1}{2\Omega}\vec{\alpha}\cdot(\vec{p}_2-\vec{p}_1)+\frac{1}{8\Omega^2}(\vec{p}_2-\vec{p}_1)^2\right] \tag{11}$$
$$\times G_0(\vec{p}_2,\vec{p}_1,\Omega_1)(\vec{\alpha}\cdot\vec{s}_2)u_{\mu_1}\left(\vec{p}_1-\vec{k}_1\right)$$

and

$$\mathfrak{M}_{\mu_1\mu_2}^{coor}(\Omega_1)=\pi\alpha Z\frac{m}{\Omega}\int_{R^3}d^3r_2u_{\mu_2}^+(\vec{r}_2)e^{-i\vec{k}_2\cdot\vec{r}_2}$$
$$\times\left[\omega(\vec{\alpha}\cdot\vec{s}_2)-\left(\vec{\alpha}\cdot\vec{k}_2\right)(\vec{\alpha}\cdot\vec{s}_2)+2\left(\vec{s}_2\cdot\vec{P}_2\right)\right] \tag{12}$$
$$\times G_0(\vec{r}_2,0;\Omega_1)\int_{R^3}d^3r_1G_0(0,\vec{r}_1;\Omega_1)$$
$$\times e^{i\vec{k}_1\cdot\vec{r}_1}(\vec{\alpha}\cdot\vec{s}_1)u_{\mu_1}(\vec{r}_1)$$

The function $G_0\left(p_2, p_1, \Omega\right)$ which occurs in the eq. (11) has the same expression as the nonrelativistic coulombian Green functions due to Schwinger [8] but its parameters τ and X are given by. eq. (7).

That means that the amplitude (11) obeys the relativistic kinematics.

For a filled K shell the Rayleigh matrix element *per electron* is expressed in terms of only two invariant amplitudes,

$M\left(\Omega\right)$ and $N\left(\Omega\right)$, so that the matrix element may be written

$$\mathfrak{M}\left(\Omega,\theta\right)=\left(\vec{s}_1\cdot\vec{s}_2\right)M\left(\Omega,\theta\right)+\left(\vec{s}_1\cdot\vec{v}_2\right)\left(\vec{s}_2\cdot\vec{v}_1\right)\times N\left(\Omega,\theta\right) \qquad (13)$$

with $\nu_1=\vec{k}_1/\omega$, $\nu_2=\vec{k}_2/\omega$ and θ is the scattering angle, $\cos\left(\theta\right)=\vec{v}_1\vec{v}_2$.

3 Minimizing the number of high transcendental functions involved in the imaginary part of the two photon elastic amplitudes

By inspecting the expressions of the invariant amplitudes in the momentum space [3] [4], we may group several integrals with the same *b* parameter so that we may put in evidence the following types of integrals introduced by the integral representation of the Green function $G\left(\vec{p}_1,\vec{p}_2,\Omega\right)$ that may be expressed in terms of Appell functions:

$$\int_0^1 d\rho\frac{\rho^{b-1-\tau}}{\left[\left(1-x_1\rho\right)\left(1-x_2\rho\right)\right]^b} = \frac{F_1\left(b-\tau;b,b;b+1-\tau;x_1,x_2\right)}{b-\tau};b=2,3... \qquad (14)$$

$$\int_0^1 d\rho\frac{\rho^{b-2-\tau}\left(1\pm\rho^2\right)}{\left[\left(1-x_1\rho\right)\left(1-x_2\rho\right)\right]^b} = \frac{F_1\left(b-1-\tau;b,b;b-\tau;x_1,x_2\right)}{b-1-\tau} \pm\frac{F_1\left(b+1-\tau;b,b;b+2-\tau;x_1,x_2\right)}{b+1-\tau};b=2,3... \qquad (15)$$

All these expressions present specific relationships between the parameters, being very convenient for their analytically properties.

Indeed, we are able to proof that the second integral may be written in the following form:

$$\begin{aligned}\int_0^1 d\rho\rho^{b-1-\tau}\frac{1\pm\rho^2}{\left[\left(1-x_1\rho\right)\left(1-x_2\rho\right)\right]^{b+1}} &= \frac{s}{2u}\left(u\pm\frac{1}{u}\right)\\ &\times\frac{F_1\left(b+1-\tau;b+1,b+1,b+2-\tau;x_1,x_2\right)}{b+1-\tau}\\ &+\frac{1}{2u}\left[\left(u\pm\frac{1}{u}\right)+\frac{\tau}{b}\left(u\mp\frac{1}{u}\right)\right]\\ &\times\frac{F_1\left(b-\tau;b,b,b+1-\tau;x_1,x_2\right)}{b-\tau}+\\ &+\left(u\mp\frac{1}{u}\right)\times\frac{\left(1-s+u^2\right)^{-b}}{2bu};b=1,2,3...\end{aligned} \qquad (16)$$

where $s=x_1+x_2$ which depends both of the photon energy and scattering angle θ and $u=\left(x_1x_2\right)^{1/2}$, which depends only on the energy.

It reveals a recurrence relationship allowing to obtain the Appell functions of the second type in terms of two Appell functions of the first type, with $b_1=b_2=b=\mathrm{Re}\left[a\right]$ and $c=a+1$.

This makes possible to minimize the number of Appell functions to be handled in the integrand. Thus, there are three Appell functions for the first type integral, and four for the second. Using the recurrence relationships we may eliminate the last four of these Appell functions.

Moreover, we may use them in connection with another specific relationship for this kind of Appell functions so that we could obtain directly the imaginary part of the amplitude (necessary for photoeffect and pair production cross sections) in terms of Gauss hypergeometric functions:

$$\begin{aligned}\mathrm{Im}\left\{\frac{X}{D^{2b}}\frac{F_1\left(b-\tau;b,b;b+1-\tau;x_1,x_2\right)}{\left(b-\tau\right)}\right\} &=\frac{\left(-1\right)^{b+1}}{\left(2b-1\right)!}\frac{\pi\alpha Z\left|\Omega\right|\varepsilon\left(x,y\right)}{2\sinh\left(\pi\left|\tau\right|\right)}\\ &\times\frac{\left(1+\left|\tau\right|^2\right)\left(4+\left|\tau\right|^2\right)...\left[\left(b-1\right)^2+\left|\tau\right|^2\right]}{\left|D\right|^{2b}}\\ &\times{}_2F_1\left(b-\tau,b+\tau;b+\frac{1}{2};v\right),b=1,2,3...\end{aligned} \qquad (17)$$

where

$$\varepsilon(x,y) = e^{|\tau|\chi_0(x,y)} = e^{|\tau|\chi_0(x)} e^{|\tau|\chi_0(y)} \tag{18}$$

$$e^{|\tau_1|\chi_0(x)} = \begin{cases} e^{-\frac{\pi}{2}|\tau_1|} e^{|\tau_1|\arctan\left[\alpha Z \frac{|X_1|}{\omega} \frac{1+x}{\gamma - \alpha^2 Z^2 \frac{m}{\omega} - \frac{\alpha^2 Z^2}{2}\frac{m}{\omega}\left(x^2+2x\right)}\right]} \\ \quad if\ x < x_0 = \left(\frac{2\gamma}{\alpha^2 Z^2}\frac{\omega}{m} - 1\right)^{1/2} - 1 \\ e^{\frac{\pi}{2}|\tau_1|} e^{-|\tau_1|\arctan\left[\alpha Z \frac{|X_1|}{\omega} \frac{1+x}{-\gamma + \alpha^2 Z^2 \frac{m}{\omega} + \frac{\alpha^2 Z^2}{2}\frac{m}{\omega}\left(x^2+2x\right)}\right]} \\ \quad if\ x \ge x_0 \end{cases} \tag{19}$$

$$e^{|\tau_2|\chi_0(x)} = e^{-\frac{\pi}{2}|\tau_2|} e^{|\tau_2|\arctan\left[\alpha Z \frac{|X_2|}{\omega} \frac{1+x}{\gamma + \alpha^2 Z^2 \frac{m}{\omega} + \alpha^2 Z^2 \frac{m}{\omega}\left(x^2+2x\right)}\right]} \tag{20}$$

It may be shown that

$$u^2 = \frac{D^{*2}(x,y)}{D^2(x,y)} = \frac{D^{*2}(x) D^{*2}(y)}{D^2(x) D^2(y)}$$

with

$$D^2(x,y) = D^2(x) D^2(y);$$

$$D^2(x) = (\lambda + X)^2 + \omega^2;\ D^2(y) = (\mu + X)^2 + \omega^2$$

$$\lambda = \lambda_0(1+x),\ \mu = \lambda_0(1+y) \tag{21}$$

and the argument of the Gauss hypergeometric function is $v = -|v| = \frac{1}{2}\left(1 - \frac{s}{2u}\right)$

This overall minimization of the number of transcendental functions is very important for implementing the expressions of the amplitude in a standard programming environment (C or Fortran). For the same purpose, we were able to further express all the hypergeometric functions that occur in terms of elementary functions using the following relationships

$$_2F_1\left(1-\tau, 1+\tau; \frac{3}{2}; v\right) = \frac{1}{\sqrt{\frac{s^2}{4u^2-1}}} \frac{\sin(w)}{|\tau|} \tag{22}$$

$$_2F_1\left(2-\tau, 2+\tau; \frac{5}{2}; v\right) = \frac{3}{4}\frac{1}{|v|}\frac{1}{1+|v|}\frac{1}{1+|\tau|^2}$$
$$\times\left[\frac{1+2|v|}{2\sqrt{|v|(1+|v|)}}\frac{\sin w}{|\tau|} - \cos w\right] \tag{23}$$

$$_2F_1\left(3-\tau, 3+\tau; \frac{7}{2}; v\right) = \frac{15}{4}\frac{1}{|v|(1+|v|)^2}\frac{1}{4+|\tau|^2}$$
$$\times\left\{(1+2|v|)\,{}_2F_1\left(2+\tau; 2-\tau; \frac{5}{2}; v\right) - \frac{1}{2}\right. \tag{24}$$
$$\left.\times\frac{1}{\sqrt{|v|(1+|v|)}}\frac{\sin w}{|\tau|}\right\}$$

where $w(\theta) = |\tau|\ln\left[1 + 2|v| + 2\sqrt{|v|(1+|v|)}\right]$.

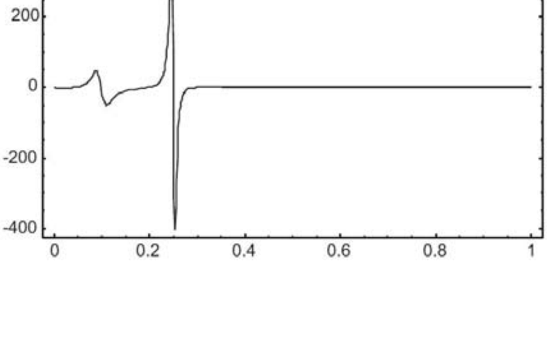
Also, the contribution of the integral in the coordinate space to the second iteration to the main term of the amplitude may be expressed in terms of two integrals that lead to Gauss hypergeometric functions:

$$M(\Omega,\theta) = \pm\pi\alpha Z\frac{m\omega}{\Omega}\left(R(\Omega) \mp \frac{\alpha Z}{1+\gamma}R'(\Omega)\right)$$
$$\times\left[R(\Omega) \mp \frac{\alpha Z}{1+\gamma}R'(\Omega) \pm 2\frac{\alpha Z}{1+\gamma}R'(\Omega)\sin^2\frac{\theta}{2}\right] \tag{25}$$

with

$$R(\Omega) = \frac{4\pi}{\omega}\int_0^\infty dr a(r) G_0(r,0;\Omega)\sin(\omega r) r;$$

$$R'(\Omega) = \frac{4\pi}{\omega}\int_0^\infty dr a(r) G_0(r,0;\Omega) r \tag{26}$$
$$\times\left[\cos(\omega r) - \frac{\sin(\omega r)}{\omega r}\right]$$



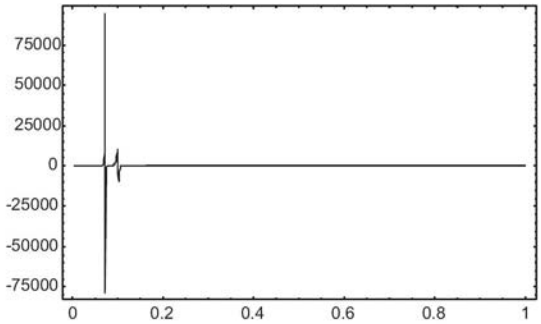


Fig. 1 The real part of the integrand of Appell function in the case of forward Rayleigh scattering for $b_1 = b_2 = 2$, $a = 1 - i|\tau|$. The first graphics corresponds to the variables values $\mathrm{Re}[x_1] = 0.1$, $\mathrm{Re}[x_2] = 1$, and the second one is for $\mathrm{Re}[x_1] = 14$, $\mathrm{Re}[x_1] = 10$

We have performed analytically the integrals $R(\Omega)$ and $R'(\Omega)$ and we have obtained the result:

$$R(\Omega) = N_0 \frac{\Gamma(1-\tau)\Gamma(\gamma+1)}{\Gamma(\gamma+1-\tau)} \\ {}_2F_1(\gamma,\gamma+1;\gamma+1-\tau;z_-) \\ -{}_2F_1(\gamma,\gamma+1;\gamma+1-\tau;z_+) \tag{27}$$

$$R'(\Omega) = N_0 \frac{\Gamma(1-\tau)\Gamma(\gamma+1)}{\Gamma(\gamma+1-\tau)} \\ \times\left[{}_2F_1(\gamma,\gamma+1;\gamma+1-\tau;z_-) \right. \\ \left. -{}_2F_1(\gamma,\gamma+1;\gamma+1-\tau;z_+)\right] \\ -\frac{2|X|}{\omega(1-\gamma)} \frac{\Gamma(1-\tau)\Gamma(\gamma)}{\Gamma(\gamma-\tau)} \\ \times\left[{}_2F_1(\gamma-1,\gamma;\gamma-\tau;z_-) \right. \\ \left. -{}_2F_1(\gamma-1,\gamma;\gamma-\tau;z_+)\right] \tag{28}$$

where

$$N_0 = \left[\frac{\lambda_0^3}{\pi}\frac{1+\gamma}{\Gamma(2\gamma+1)}\right]^{1/2} \frac{-1}{4\omega|X|}\left(\frac{\lambda_0}{X}\right)^{\gamma-1}\Gamma(\gamma);$$

$$z_\pm = \frac{1}{2|X|}\left(|X| \pm \omega - i\lambda\right) \tag{29}$$

and ${}_2F_1(a,b,c;z)$ is the Gauss hypergeometric function (GHF).

We point out that all GHF involved in the right side of the eq. 28 present simple relationships among the parameters $b - a = 1$ and $c - a = 1 - \tau$. For such functions we may write:

$$\frac{1}{\gamma-1}\frac{\Gamma(\gamma)\Gamma(1-\tau)}{\Gamma(\gamma-\tau)}\,{}_2F_1(\gamma-1,\gamma;\gamma-\tau;z) \\ = \frac{1}{\gamma-1}\frac{1}{(-z)^{\gamma-1}} + \frac{\tau\ln(-z)}{(-z)^\gamma}\left(\frac{-z}{1-z}\right)^{\gamma+\tau-1} \\ \times{}_2F_1\left(2-\gamma,1-\tau;2;\frac{1}{z}\right) - \frac{1}{(-z)^\gamma}\frac{\pi|\tau|}{\tanh(\pi|\tau|)} \\ \times{}_2F_1\left(\gamma,1+\tau;2;\frac{1}{z}\right) + \frac{\tau}{(-z)^\gamma}\sum_{n=0}^{\infty}\frac{(\gamma)_n}{n!}\frac{(1+\tau)_n}{(n+1)!} \\ \times\left(\frac{1}{z}\right)^n\left\{\frac{1}{n+1} + \psi(n+1) - \psi(n+\gamma) - \tau \right. \\ \left. \times\sum_{k=n+1}^{\infty}\frac{k-\tau}{k\left(k^2+|\tau|^2\right)}\right\} \tag{30}$$

where $\psi(z)$ is the logarithmic derivative of $\Gamma(z)$ function.

4 Analytical treatment of the real part of the amplitude

The following relationship may be used for expressing the Appell functions in terms of HGF

$$F_1(a;b,b;c;x_1,x_2) = (1-u)^{c-a-2b} \\ \times\sum_{p=0}^{\infty}\frac{(a)_p(b)_p}{(c)_p\,p!}\left[\frac{s-2u}{(1-u)^2}\right]^p \\ \times{}_2F_1(c-a,c-2b-p;c+p;u) \tag{31}$$

with $s = x_1 + x_2$, $u = (x_1x_2)^{\frac{1}{2}} \equiv \dfrac{D^*}{D}$

In our case $c = a+1$, $a = d - \tau$ and one may demonstrate that

$$1-u = \frac{D^2 - D^{*2}}{2|D|^2} - \left(\frac{D^2 + D^{*2}}{2|D|^2} - 1\right) \tag{32}$$

We will try to reduce the appearing HGF to a form that is more convenient in order to take advantage of the relationship

$${}_2F_1(1,-\tau;2-\tau;u) = 1 + \mathcal{O}(\alpha Z) \tag{33}$$

This allows us to eliminate the terms in a higher order of αZ from the expressions of the amplitudes, taking in consideration the small value of Sommerfeld constant, $\alpha \approx 1/137$.

We may write the following recurrence relationships between the HGF that occur in the expressions of amplitude

$$\frac{p+1}{2+p-\tau}\,{}_2F_1(1,-p-1-\tau;3+p-\tau;u)$$
$$=\frac{1+p}{2(3+2p)}\left(\frac{D^2+D^{*2}+2|D|^2}{2|D|^2}+\frac{D^2-D^{*2}}{2|D|^2}\right)$$
$$+\frac{\tau}{2(3+2p)}\frac{D^2-D^{*2}}{2|D|^2}\left[1+\frac{D^2-D^{*2}}{D^2+D^{*2}+2|D|^2}\right] \quad (34)$$
$$-\frac{1+p+\tau}{2(3+2p)}\frac{\left(D^2-D^{*2}\right)^2}{D^2+D^{*2}+2|D|^2}$$
$$\times\frac{{}_2F_1(1,-p-\tau;2+p-\tau;u)}{|D|^2}$$

$$\frac{p+2}{3+p-\tau}\,{}_2F_1(1,-p-2-\tau;4+p-\tau;u)$$
$$=\frac{2+p+\tau}{2(5+2p)}\frac{\left(D^2-D^{*2}\right)^2}{D^2+D^{*2}+2|D|^2}\frac{1}{|D|^2}$$
$$\times\frac{{}_2F_1(1,-p-\tau;2+p-\tau;u)}{|D|^2}+ \quad (35)$$
$$\frac{1}{2(5+2p)}\left(\frac{2+p+\tau}{u}+2+p-\tau\right)$$

$$\frac{p+1}{2+p-\tau}\,{}_2F_1(1,-p-1-\tau;3+p-\tau;u)$$
$$=\frac{1+p+\tau}{2(3+2p)}\frac{\left(D^2-D^{*2}\right)^2}{D^2+D^{*2}+2|D|^2}\frac{1}{|D|^2}$$
$$\times\frac{{}_2F_1(1,-p-\tau;2+p-\tau;u)}{|D|^2}+ \quad (36)$$
$$\frac{1}{2(3+2p)}\left[(1+p)\frac{1+u}{u}+\tau\frac{1-u}{u}\right]$$

where

$$\frac{1+u}{u}=\frac{D^2+D^{*2}}{2|D|^2}+\frac{D^2-D^{*2}}{2|D|^2}+1$$
$$\frac{1-u}{u}=\frac{D^2+D^{*2}}{2|D|^2}+\frac{D^2-D^{*2}}{2|D|^2}-1$$

As the physical conditions prove, most of the terms with $p\geq 1$ have a higher order in αZ than the rest of the terms in the real part of the expression of the scattering amplitude.

Using the relationships (33) and (34), for $p=0$ it follows

$$\frac{1}{2-\tau}\,{}_2F_1(1,-1-\tau;3-\tau;u)$$
$$=\frac{1}{6}\left(\frac{D^2+D^{*2}}{2|D|^2}+1+\frac{D^2-D^{*2}}{2|D|^2}\right) \quad (37)$$
$$+\frac{\tau}{6}\frac{D^2-D^{*2}}{2|D|^2}-\frac{\tau}{6|D|^2}\frac{\left(D^2-D^{*2}\right)^2}{D^2+D^{*2}+2|D|^2}$$
$$+\mathcal{O}(\alpha^3Z^3)$$

The term $\frac{D^2-D^{*2}}{2|D|^2}$ has no contribution to the real part of the amplitude when multiplied by 1, but it does contribute when multiplied with $\frac{D^2-D^{*2}}{D^2+D^{*2}+2|D|^2}$.

Thus, the relationship (31) becomes:

$$\frac{1}{D^4}\frac{F_1(2-\tau;2,2;3-\tau;s,u)}{2-\tau}=\frac{1}{\left(D^2-D^{*2}\right)^3}$$
$$\left[1+\frac{D^2-D^{*2}}{D^2+D^{*2}+2|D|^2}\right]\frac{D^2+D^{*2}+2|D|^2}{2|D|^2} \quad (37)$$
$$\times\sum_{p=0}^{\infty}(1+p)\left\{1-\frac{1}{4}\left[1+\frac{\vec{\Delta}^2}{(\lambda+\mu)^2}\right]\frac{D^2+D^{*2}+2|D|^2}{(X^2+\omega^2+\lambda\mu)^2}\right\}^p$$
$$\times\frac{{}_2F_1(1,-1-p-\tau;3+p-\tau;u)}{2+p-\tau}$$

Taking into account the relationship (33) it follows that if we are interested in obtaining the real part of the amplitude up till $(\alpha Z)^4$, the sum in (37) may be truncated at the first term as the others are in $(\alpha Z)^5$.

Indeed, from the physical parameter of the process one may see that

$$D^2+D^{*2}+2|D|^2=4(X^2+\omega^2+\lambda\mu)^2$$
$$+\mathcal{O}(\alpha^4Z^4x^4) \quad (38)$$

which reveals the higher order of the rest of the terms in equation (37)

5 Numerical results

We applied all these calculations for obtaining the full relativistic expressions of forward Rayleigh scattering amplitudes in the order $(\alpha Z)^4$ for the real part and in the order $(\alpha Z)^7$ in the imaginary part.

The recurrence relationships (15), (16) allow the minimization of the number of necessary Appell functions, while the relationships (17) and (22-24) allow in some cases to express them in terms of less transcendental functions.

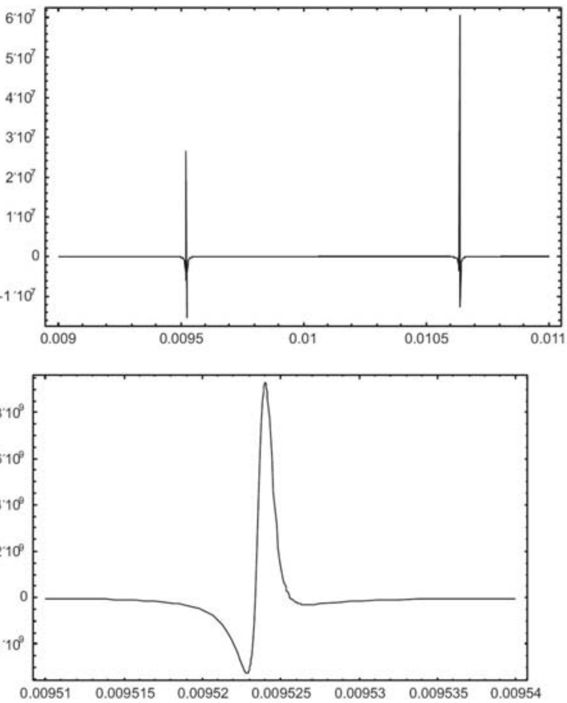


Fig. 2 The real part of the integrand of Appell function in the case of forward Rayleigh scattering for $b_1 = b_2 = 2$, $a = 1 - |\tau|$ and $\mathrm{Re}[x_1] = 94$, $\mathrm{Re}[x_2] = 105$ *(upper figure)*. The same integrand focused on the first "pathological" region *(lower figure).*

This opportunity has a great impact on the overall computing effort in the final numerical calculations, as the higher transcendental functions are very difficult to estimate due to the almost "pathological" nature of the integrand in many cases, especially in the vicinity of the physical thresholds [7].

From figure 1 one may see that the integrand of the Appell function has a well behaved aspect for low values of the real part of the variables and become more and more pathological for larger values, which occur especially in the high photon energy regime. Also, the parameter τ tends to infinity at the physical threshold energies. This aspect make very difficult the use of standard boxed quadrature programs, as the region with significant values of the integrand is very narrow. In the general case of Appell functions with different values of the variables there are two poles that abruptly amplify the oscillating numerator (as its exponent is complex above the threshold).

The solution for managing the quadrature in these cases is to notice that only two narrow vicinities of $\frac{1}{x_1}$ and $\frac{1}{x_1}$ have to be considered and, as it is shown in figure 2, a standard quadrature may be very accurate in these regions, without a huge computational effort.

The validity of this technique was checked by including it in the calculation of the photoeffect cross sections in the high energy regime and by comparing our results with other published ones. The photoeffect cross sections were obtained via the optical theorem from the imaginary part of the forward Rayleigh scattering amplitude:

$$\sigma_{ph} = 4\frac{\pi}{\alpha}\frac{m}{\omega} r_0^2 \,\mathrm{Im}[A] \tag{31}$$

The comparison of our numerical results for the photoeffect cross sections up to several MeV with similar results of Scofield [9] and Kissell *et al* [10] showed a very good agreement, within 3% even for heavy elements at photon energies where the relativistic effects are important.

In figures 3-6 we present the numerical results obtained with the above relationships in the nonrelativistic limit [2] for the angular distribution of the Rayleigh scattering of X rays on the K-shell various elements, for incoming photon energy under the threshold. One may notice that the forward scattering is lower than the back scattering if the threshold energy is much greater than the photon energies (figures 3 and 4). Also a reversed situation occurs when the photon energy is closer to the target's threshold energy (figure 6).

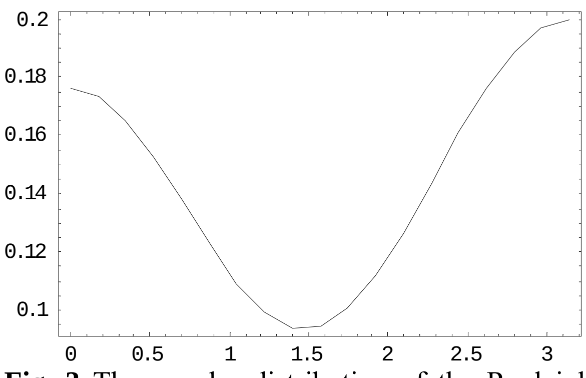


Fig. 3 The angular distribution of the Rayleigh scattering cross section of K-shell

electrons for Z=92 at 50 keV

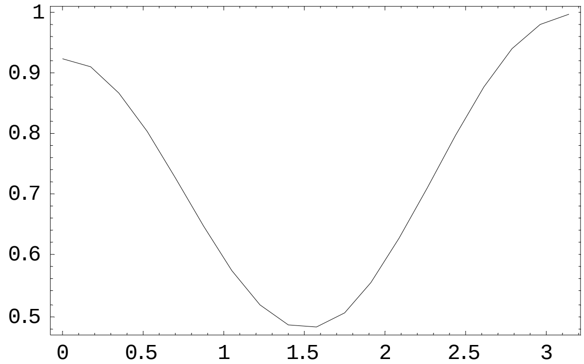


Fig. 4 The angular distribution of the Rayleigh scattering cross section of K-shell electrons for Z=82 at 50 keV

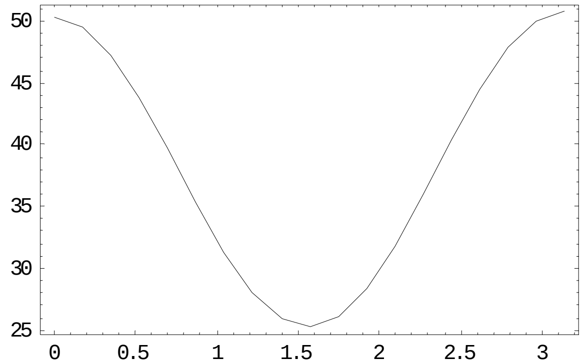


Fig. 5 The angular distribution of the Rayleigh scattering cross section of K-shell electrons for Z=70 at 50 keV

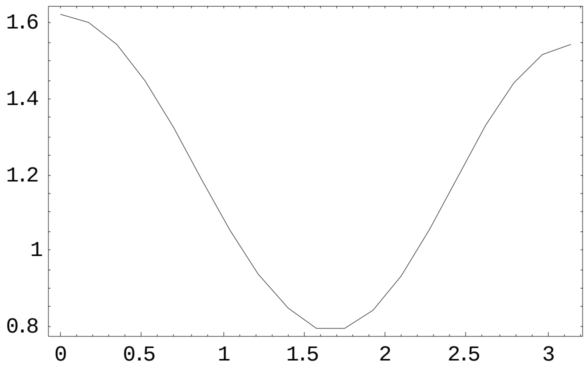


Fig. 6 The angular distribution of the Rayleigh scattering cross section of K-shell electrons for Z=70 at 50 keV

We also present in Table 1 and Table 2 the numerical values of the angular distribution of the Rayleigh scattering cross section and the real parts of the perpendicular and parallel components of the amplitude for the K-shell electrons of medium atomic number elements. It is obvious that for lower photon energy and not too high atomic number the angular distribution tends to be symmetric, since the retardation, multipole and spin effects become negligible.

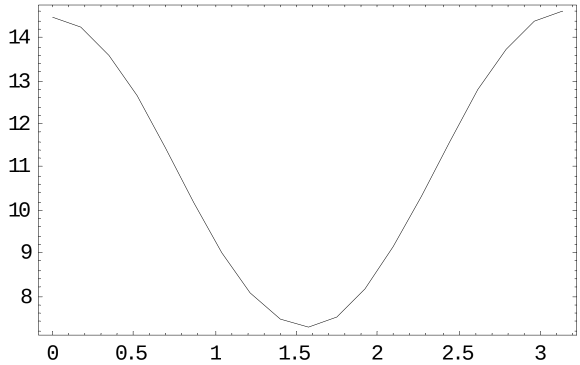


Fig. 7 The angular distribution of the Rayleigh scattering cross section of K-shell electrons for Z=47 at 20 keV

Table 1. Angular distribution of the Rayleigh scattering cross section and the real parts of the perpendicular and parallel components of the amplitude for the K-shell electrons of Ag at 25 keV.

Angle (deg)	S (barn)	Re[Aperp]	Re[Apar]
0	35.7547	2.12208	2.12208
10.	35.2257	2.12208	2.09044
20.	33.7008	2.12211	1.99642
30.	31.359	2.12215	1.84273
40.	28.4762	2.1222	1.63379
50.	25.3932	2.12227	1.37563
60.	22.4767	2.12236	1.0758
70.	20.0761	2.12246	0.743099
80.	18.4817	2.12258	0.387398
90.	17.8895	2.12271	0.0193509
100.	18.3764	2.12284	-0.349909
110.	19.8888	2.12298	-0.709101
120.	22.248	2.12312	-1.04715
130.	25.1703	2.12325	-1.35355
140.	28.3007	2.12336	-1.61868
150.	31.2564	2.12346	-1.83419
160.	33.6741	2.12353	-1.99323
170.	35.2557	2.12357	-2.09074
180.	35.8056	2.12359	-2.12359

If the photon energy is above the threshold energy, the relativistic effects become important especially for high Z elements. In figure 8 and figure 9 one may notice that the angular distribution is far from the symmetry predicted by older models, some of them with a very limited applicability [11-14]. In figure 9 the numerical results of Kissell *et al* [10] are also represented (with error bars) and a very good concordance may be observed even in the gamma-ray regime and high atomic number elements.

Table 2. Angular distribution of the Rayleigh scattering cross section and the real parts of the

perpendicular and parallel components of the amplitude for the K-shell electrons of Zn at 10 keV.

Angle (deg)	S (barn)	Re[Aperp]	Re[Apar]
0	38.661	2.20664	2.20664
10.	38.0826	2.20664	2.17337
20.	36.4164	2.20666	2.07454
30.	33.8612	2.20669	1.9131
40.	30.7224	2.20674	1.69385
50.	27.3754	2.20679	1.42331
60.	24.2218	2.20685	1.10957
70.	21.6408	2.20692	0.762037
80.	19.9442	2.207	0.391169
90.	19.3384	2.20707	0.0081668
100.	19.8989	2.20716	-0.375356
110.	21.5605	2.20723	-0.747722
120.	24.1245	2.20731	-1.09755
130.	27.2821	2.20738	-1.4141
140.	30.6513	2.20744	-1.68764
150.	33.8236	2.20749	-1.90971
160.	36.4134	2.20752	-2.07344
170.	38.1053	2.20755	-2.17376
180.	38.6932	2.20756	-2.20756

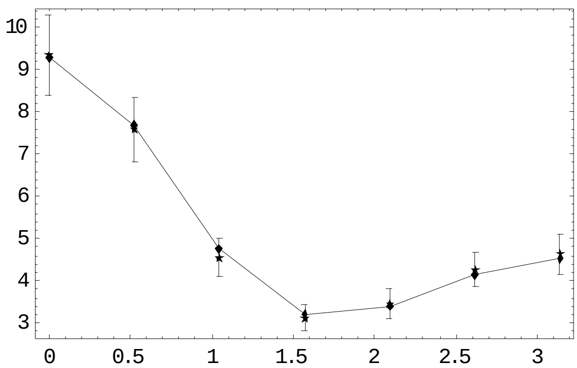


Fig. 8 The angular distribution of the Rayleigh scattering cross section of K-shell electrons for Z=82 at 160 keV

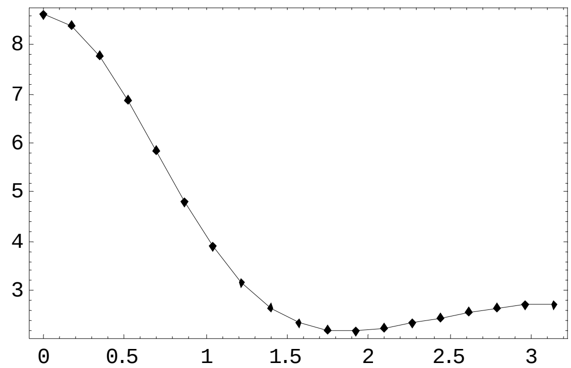


Fig. 9 The angular distribution of the Rayleigh scattering cross section of K-shell electrons for Z=82 at 200 keV

A complete set of numerical results for the Rayleigh scattering in the gamma –ray regime for K-shell electrons of lead is presented in table 3. Both the imaginary and the real parts of the perpendicular and parallel components of the amplitude show a very good agreement with other data presented in literature, proving the validity of our mathematical and physical model.

Table 3. Angular distribution of the Rayleigh scattering cross section and the real and imaginar parts of the perpendicular and parallel components of the amplitude for the K-shell electrons of Pb at 200 keV.

Angle (deg)	S(barn)	Re[Aperp]	Im[Aperp]	Re[Apar]	Im[Apar]
0	8.614	0.995	-0.306	0.995	-0.306
10	8.395	0.990	-0.305	0.975	-0.297
20	7.781	0.975	-0.300	0.919	-0.270
30	6.881	0.952	-0.293	0.829	-0.228
40	5.840	0.922	-0.283	0.712	-0.177
50	4.805	0.887	-0.271	0.577	-0.121
60	3.890	0.849	-0.259	0.432	-0.066
70	3.166	0.809	-0.246	0.284	-0.014
80	2.655	0.770	-0.233	0.140	0.030
90	2.344	0.732	-0.221	0.005	0.067
100	2.200	0.697	-0.210	-0.116	0.097
110	2.178	0.666	-0.200	-0.224	0.120
120	2.236	0.638	-0.191	-0.316	0.136
130	2.337	0.614	-0.183	-0.393	0.148
140	2.451	0.595	-0.177	-0.455	0.156
150	2.559	0.580	-0.172	-0.502	0.161
160	2.644	0.569	-0.168	-0.535	0.164
170	2.699	0.563	-0.166	-0.554	0.165
180	2.718	0.560	-0.166	-0.560	0.166

6 Conclusions

The high transcendental functions that occur in the relativistic expressions of the two-photon atomic processes may be reduced to less computer demanding functions using several recurrence relationships and identities. The specificity of the involved functions parameters has been exploited and both the imaginary and the real part of these functions have been analytically treated. This allows to minimize the number and complexity of the transcendental functions needed for amplitude calculation in $(\alpha Z)^4$ for the real part and $(\alpha Z)^7$ in the imaginary part. The numerical results obtained using the presented procedure show a very good agreement with other results in the literature.

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