Proceedings of the 8th WSEAS International Conference on APPLIED MATHEMATICS, Tenerife, Spain, December 16-18, 2005 (pp239-244)

Numerical evaluation and integration of higher transcendental Lauricella and Appell functions involved in photon-atom interactions

A. COSTESCU
Department of Physics, University of Bucharest, MG11, Bucharest-Magurele 76900, ROMANIA

S. SPANULESCU
Department of Physics, Hyperion University of Bucharest, Postal code 030629, Bucharest ROMANIA
Department of Physics, University of Bucharest, MG11, Bucharest-Magurele 76900, ROMANIA

Abstract:-The triply differential cross-section for the inelastic Compton scattering of photons by K-shell bound electrons is expressed in closed form in terms of four high transcendental Lauricella functions F_D of *four* variables and *six* parameters, all complex. In order to obtain the doubly differential cross-section, a numerical integration over the directions of the final electron is needed. The aim of this paper is to present a method for both evaluation and integration over the solid angle of Lauricella functions, valid for any photon energy and target's atomic number. While all the researchers seem to avoid even the evaluation of these functions, we present a new quadrature method, based on the analysis of the pathological behavior of the integrand near origin. Also, the solid angle integration process is achieved and discussed. Keeping the full form of the Lauricella functions allowed us to include in the doubly differential cross-section the *exact* dependence on the angles describing the directions of the final electron and photon. The accuracy of evaluating the Lauricella functions was checked by using recurrence relations between them, and a fairly good precision was observed for any physical parameters and variables occurring in two photon bound-free electron transitions. We mention that our analytical approach of the triply differential cross-section allows the numerical calculation of the doubly differential one in seconds using an average personal computer. Also, our results based on these evaluations display a good agreement with direct numerical calculations of the S-matrix element performed by Bergstrom *et al* [Phys. Rev. A 48, 1134 (1993)] on Cray computers.

Key-Words: - Lauricella, Compton cross sections, quadrature, pathological integrand, Green function, recurrence

1. Introduction

Since Schwinger [2] gave an integral representation for the Green function of the Schrodinger equation with Coulomb field, it became possible to perform analytical calculations for obtaining the nonrelativistic differential scattering amplitudes for two photon atomic processes in closed form.

Because the integration contour introduced by Schwinger's coulombian Green function is the same integral contour occurring in the integral representation of Appell and Lauricella functions, taking into account the basic sixfold integral given by Gavrila and Costescu [3], the full nonrelativistic results may be expressed in terms of these higher transcendental functions. More specific, the two photon bound-bound transitions involve Appell functions, while the more complicated case of bound-continuum transitions involves Lauricella functions $F_D(a;b_1,b_2,b_3,b_4;c;z_1,z_2,z_3,z_4)$, which could not be numerically evaluated until now, moreover integrated.

In the nonrelativistic limit of the second order S-matrix element, from rotational invariance considerations, the Compton amplitude M for photon scattering on K-shell electrons is:

$$\begin{aligned}M &= A(\vec{s}_1\vec{s}_2)+B(\vec{s}_1\vec{\nu}_2)(\vec{s}_2\vec{\nu}_1)+C(\vec{s}_1\vec{n})(\vec{s}_2\vec{\nu}_1)\\ &+D(\vec{s}_2\vec{n})(\vec{s}_1\vec{\nu}_2)+E(\vec{s}_1\vec{n})(\vec{s}_2\vec{n})\end{aligned} \qquad (1)$$

where the invariant scattering amplitudes are:

$$A=\vartheta-P(\Omega_1)-P(\Omega_2),\ E=-(T(\Omega_1)+T(\Omega_2)),$$
$$B=-(L(\Omega_1)+L(\Omega_2)), C=-R(\Omega_1)+S(\Omega_2),$$
$$D=-S(\Omega_1)+R(\Omega_2) \qquad (2)$$

with $\Omega_1=\omega_1+\gamma m$, $\Omega_2=-\omega_1+\gamma m$, $\gamma=(1-\alpha^2Z^2)^{1/2}$.

The form factor $\vartheta = [e^{i(\vec{k}_1 - \vec{k}_1)\vec{r}}]_{fi}$ in equation (2) is given by the expression [3]:

$$\vartheta = \frac{N}{8}\lambda^4\left(\vec{\Delta}^2 + (\nu-1)\,\vec{p}\,\vec{\Delta}\right)\frac{\left[\vec{\Delta}^2 + (\lambda - ip)^2\right]^{\nu-1}}{\left[(\vec{\Delta} - \vec{p})^2 + \lambda^2\right]^{\nu+2}} \qquad (3)$$

where $\vec{\Delta}$ is the photon momentum transfer, $\lambda = \alpha Z m, \nu = -i\lambda / p$, $\vec{p} = \vec{n}\,p$ is the electron momentum, and $N = 2^{\frac{11}{2}}\pi^{-1/2}\left(1 - e^{-2\pi|\nu|}\right)^{\frac{1}{2}}$.

2. The triply and doubly differential cross-sections

In the case of Compton inelastic scattering of unpolarized photons by K-shell electrons averaged over the initial and summed over the final photon polarization vectors $\vec{s}_1$, $\vec{s}_2$ we get for the triply differential cross-section the expression [4]:

$$\begin{aligned}
\frac{d^3\sigma}{d\omega_2\, d\Omega_{\vec{k}_2}\, d\Omega_{\vec{p}}} = r_0^2\,\frac{\omega_2}{\omega_1}\Bigg[&\frac{1+\cos^2\theta}{2}|A|^2 \\
&+ \mathrm{Re}(ED^*)\sin^2\theta'(\cos\theta' - \cos\theta''\cos\theta) \\
&+ \mathrm{Re}(EC^*)(\cos\theta'' - \cos\theta'\cos\theta)(1-\cos^2\theta'') \\
&+ \mathrm{Re}(CD^*)(\cos\theta' - \cos\theta''\cos\theta)(\cos\theta'' - \cos\theta'\cos\theta) \\
&+ \mathrm{Re}(BE^*)(\cos\theta' - \cos\theta''\cos\theta)(\cos\theta'' - \cos\theta'\cos\theta) \\
&+ \mathrm{Re}(BD^*)\sin^2\theta(\cos\theta'' - \cos\theta'\cos\theta) \\
&+ \mathrm{Re}(BC^*)\sin^2\theta(\cos\theta' - \cos\theta''\cos\theta) \\
&- \mathrm{Re}(DA^*)\sin\theta\cos\theta\sin\theta'\cos\varphi \\
&+ \mathrm{Re}(CA^*)\cos\theta(-\cos\theta' + \cos\theta''\cos\theta) \\
&- \mathrm{Re}(BA^*)\cos\theta\sin^2\theta + |D|^2\sin^2\theta\sin^2\theta' \\
&+ \frac{1}{2}|C|^2\sin^2\theta(1-\cos^2\theta'') + \frac{1}{2}|B|^2\sin^4\theta \\
&+ \mathrm{Re}(EA^*)(\sin^2\theta' - \sin^2\theta\sin^2\theta'\cos^2\varphi \\
&- \sin\theta\cos\theta\sin\theta'\cos\theta'\cos\varphi) + |E|^2\sin^2\theta'(1-\cos^2\theta'')\Bigg] \qquad (4)
\end{aligned}$$

where ω_1 and ω_2 are the initial and final photon energies respectively, while r_0 stands for the electron classical radius. The angles θ, θ', φ are the angles between the final and initial photons, the electron momentum and the initial photon momentum, the electron momentum and the final photon momentum, respectively. The tip of the spectrum corresponds to $\omega_{2\max} = \omega_1 - (1-\gamma)m$. Our invariant amplitudes are:

$$P = \mathcal{N}\frac{\lambda^5}{d^2 fg}F_D(2-\tau;1-\nu,1+\nu;z_1,z_2;z_3,z_4) \qquad (5)$$

$$\begin{aligned}
T = 2\mathcal{N}\,p\frac{\lambda^5(\nu+1)}{d^2g^3}\Bigg\{&iX\Bigg[z_1z_2\frac{F_D(4-\tau;1-\nu,2+\nu;z_1,z_2;z_3,z_4)}{4-\tau} \\
&-\frac{F_D(2-\tau;1-\nu,2+\nu;z_1,z_2;z_3,z_4)}{2-\tau}\Bigg] \qquad (7)\\
&+p\frac{F_D(2-\tau;-\nu,1+\nu;z_1,z_2;z_3,z_4)}{2-\tau} + \\
&+\frac{p}{\tau}(1-z_1-z_2+z_1z_2)^{\nu}(1-z_3-z_4+z_3z_4)^{-2-\nu}\Bigg\}
\end{aligned}$$

$$\begin{aligned}
L = 8\mathcal{N}X^2\frac{\lambda^5\omega_1\omega_2}{d^3fg}\Bigg\{&\frac{\nu+1}{g}\frac{F_D(3-\tau;1-\nu,2+\nu;z_1,z_2;z_3,z_4)}{3-\tau} \qquad (6)\\
&-\frac{\nu-1}{f}\frac{F_D(3-\tau;2-\nu,1+\nu;z_1,z_2;z_3,z)}{3-\tau}\Bigg\}
\end{aligned}$$

$$R = 8\mathcal{N}X^2\frac{\lambda^5p\omega(\nu+1)}{d^3fg^2}\frac{F_D(3-\tau;1-\nu,2+\nu;z_1,z_2;z_3,z_4)}{3-\tau} \qquad (8)$$

$$\begin{aligned}
S = 2\mathcal{N}\frac{\omega_1\omega_2}{\omega_j}\frac{\lambda^5(\nu+1)}{d^2g^2}\Bigg\{&iX\left(\frac{z_1z_2}{g} - \frac{1}{f}\frac{d^*}{d}\right)\Bigg[\frac{F_D(4-\tau;1-\nu;2+\nu;z_1,z_2;z_3,z_4)}{4-\tau} \\
&+iX\left(\frac{1}{f} - \frac{1}{g}\right)\frac{F_D(2-\tau;1-\nu;2+\nu;z_1,z_2;z_3,z_4)}{2-\tau}\Bigg] \qquad (9)\\
&+\frac{p}{g}\frac{F_D(2-\tau_j;-\nu;2+\nu;z_1,z_2;z_3,z_4)}{2-\tau} + \frac{p}{\tau g}(1-z_1-z_2+z_1z_2)^{\nu}(1-z_3-z_4+z_3z_4)^{-2-\nu}\Bigg\}
\end{aligned}$$

where

$$\tau = \frac{\lambda}{X}, X_1 = -i\sqrt{2m\omega_{2\max}}, X_2 = \sqrt{2\gamma m\omega_2 + \alpha^2Z^2m^2},$$

$$f(\Omega_1) = -4m\omega_{2\max}\left(1 - \frac{\omega_2}{2\omega_{2\max}} + \sqrt{1 - \frac{\omega_2}{\omega_{2\max}}}\right),$$

$$f(\Omega_2) = 2m\omega_1 e^{-i\chi_2}, \qquad d(\Omega_1) = 2m\omega_1 e^{-i\chi_0},$$

$$d(\Omega_2) = 2m\omega_2\left(\gamma + \frac{\alpha^2Z^2m}{\omega_2}\right) + \alpha Z\sqrt{\frac{m}{\omega_2}}\sqrt{2\gamma + \frac{\alpha^2Z^2m}{\omega_2}},$$

$$g(\Omega_1) = -2m\omega_2\left(1 - \frac{p}{m}\cos\theta''\right), g(\Omega_2) = 2m\omega_1\left(1 - \frac{p}{m}\cos\theta'\right)$$

with phases χ_0 and χ_2 not depending on the angles. The Lauricella functions variables are:

$$z_1(\Omega_1) + z_2(\Omega_1) = 4\frac{\omega_2}{m}\frac{m^2 - 2X_1^2\sin^2\frac{\theta}{2}}{f(\Omega_1)}e^{i\chi_0},$$

$$z_1(\Omega_2) + z_2(\Omega_2) = 4\frac{\omega_2}{m}\frac{m^2 - 2X_2^2\sin^2\frac{\theta}{2}}{d(\Omega_2)}e^{i\chi_2},$$

$$\begin{aligned}
z_3(\Omega_1) + z_4(\Omega_1) = \Bigg[&2\frac{\Omega_1}{m}\left(1 - 2\frac{X_1^2}{g(\Omega_1)}\right) \\
&+4\frac{X_1^2}{g(\Omega_1)}\frac{\omega_2\cos\theta + p\cos\theta''}{m}\Bigg]e^{i\chi_0},
\end{aligned}$$

$$z_3(\Omega_2)+z_4(\Omega_2)=-4\Omega_2\frac{\omega_2}{d(\Omega_2)}\left(1-2\frac{X_2^2}{g(\Omega_2)}\right)$$
$$+8\frac{X_2^2}{g(\Omega_2)}\frac{\omega_2}{d(\Omega_2)}\left(\omega_1\cos\theta-p\cos\theta'\right),$$
$$z_1(\Omega_1)z_2(\Omega_1)=\frac{4m^2\omega_2^2}{f^2(\Omega_1)}e^{2i\chi_0},\ z_1(\Omega_2)z_2(\Omega_2)=\frac{4m^2\omega_2^2}{d^2(\Omega_2)}e^{2i\chi_2},$$
$$z_3(\Omega_1)z_4(\Omega_1)=e^{2i\chi_0},\ z_3(\Omega_2)z_4(\Omega_2)=\frac{4m^2\omega_2^2}{d^2(\Omega_2)},$$
$$\mathcal{N}=NX^3\left(\frac{f(\Omega)}{g(\Omega}\right)^{\nu}.$$

Integrating the triply differential cross-section over the final electron momentum direction one gets the doubly differential cross-section for Compton scattering:

$$\frac{d^2\sigma}{d\Omega_{k_2}d\omega_2}=\frac{1}{2}\int_{\Omega_p}\sum_{\vec{s}_1,\vec{s}_2}|M|^2 d\Omega\frac{\omega_2}{\omega_1}r_0^2 \tag{10}$$

Inspecting the relations (1.1) - (1.8) we observe that the integral (1.9) requires a double integration over a product of two Lauricella functions, which include the cumbersome angle dependence involved in their arguments. It is quite obvious that is not possible to perform any further analytical integration but only a numerical one.

3. Numerical evaluation and integration of the product of two Lauricella functions

The integral representation of Lauricella function is (for $\mathrm{Re}\,a>0$ and $\mathrm{Re}(c-a)>0$):

$$F_D(a;b_1,b_2,b_3,b_4;c;z_1,z_2,z_3,z_4)=-\frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)}\left(\frac{ie^{-i\pi a}}{2\sin\pi a}\right)\int_1^{(0+)}\frac{\rho^{a-1}(1-\rho)^{c-a-1}}{(1-\rho z_1)^{b_1}(1-\rho z_2)^{b_2}(1-\rho z_3)^{b_3}(1-\rho z_4)^{b_4}}d\rho \tag{11}$$

where the integration contour begins from the point $1+i\varepsilon$ in the upper semiplane of the complex variable ρ and ends in the point $1-i\varepsilon$ in the lower semiplane, encircling the origin in counter-clockwise sense.

Inspecting the parameters of the Lauricella functions we need, and comparing with the integral representation (2.1) one observes that the relationship $c=a+1$ holds for all these functions. In this case, there is no cut between the origin and the point 1 so that the integral representation (2.1) becomes:

$$F_D(a;b_1,b_2,b_3,b_4;a+1;z_1,z_2,z_3,z_4)=a\int_0^1\frac{\rho^{a-1}}{(1-\rho z_1)^{b_1}(1-\rho z_2)^{b_2}(1-\rho z_3)^{b_3}(1-\rho z_4)^{b_4}}d\rho;\qquad \mathrm{Re}\,a>0; \tag{12}$$

The main difficulty for calculating the Lauricella function F_D in the integral representation comes from its large number of parameters, giving a large variety of shapes of the integrand. Many of them are pathological, with regions of very fast variations combined with slow variation regions. It is very challenging for all standard quadrature methods, which fail to converge in many situations, or have a poor rate of approximation.

However, inspecting the shape of the integrand, it comes out that the fast variation regions are concentrated in the vicinity of the origin, producing important truncation errors. Obviously, the ρ^a term (a being complex) has an oscillating behavior with the frequency $f=\frac{|\mathrm{Im}(a)\ln\rho|}{2\pi}$, revealing a very difficult quadrature when ρ tends to 0.

Figures 1-3 show that the shape of the integrand for some important physical situations of the Compton scattering theory where they are involved. One may observe that both the real and the imaginary part of the integrand are highly oscillating, so any standard sampling method of the whole interval [0, 1] is inadequate. Indeed, the other methods for sampling the integrand, with equidistant or Gauss points [6,7] will treat equally the edges of the integration domain, not allowing to have a much greater number of points in the difficult region.

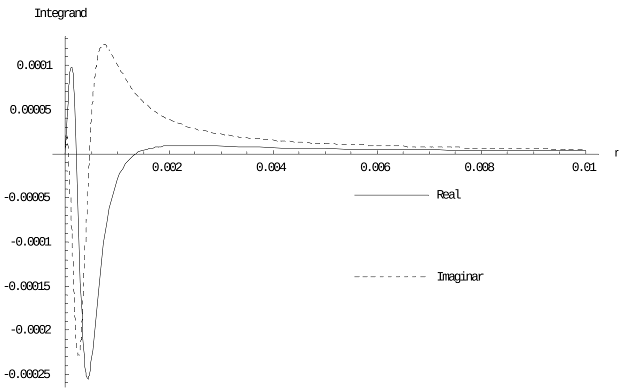

FIG. 1 - Lauricella integrand for Compton scattering at 150keV, Z=30, θ=60°

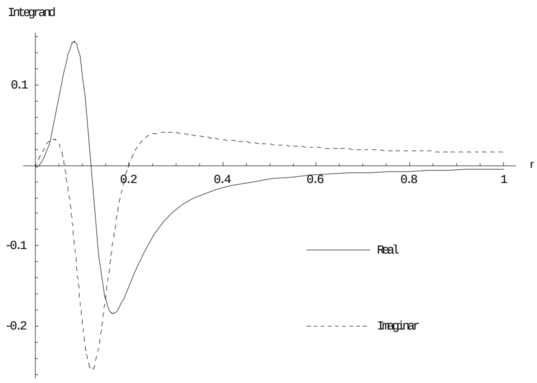

FIG. 2 - Lauricella integrand for Compton scattering at 661keV, Z=82, θ=0°

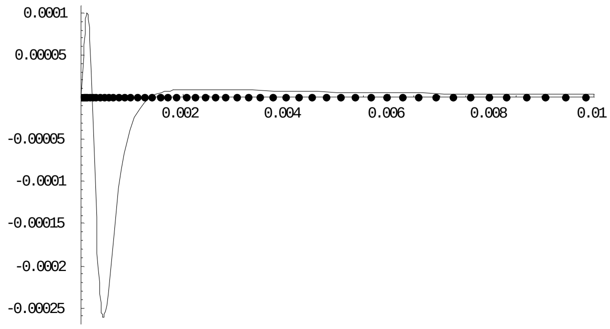

FIG 3. Sampling points for quadrature

For accurately evaluating the Lauricella functions, we propose a procedure with an increasing sampling rate, in a continuous or discontinuous way, when approaching the origin, followed by a mid-point quadrature.

We point out that the same difficulty also occurs when calculating the integral representations of hypergeometric Gauss function ${}_2F_1(a,b;c;z)$ and Appell function $F_1(a;b_1,b_2;c;z_1,z_2)$, but with a significantly simpler behavior of the denominator, so our method may be used for these cases too.

A simple yet efficient way for variable sampling the interval may be chosen in a linear form as:

$$\Delta x_i = a + b(i-1) \tag{13}$$

where Δx_i is the width of the *i*th interval, *a* is the width of the first interval (chosen by us between 10^{-4} and 10^{-6}) and *b* results from the upper limit of the domain:

$$\sum_{i=1}^{N} \Delta x_i = 1 \ ; \ b = 2\frac{1/N - a}{N-1}$$

where *N* is the number of intervals.

The integrand should be evaluated in the middle of each of the N intervals $x_{km} = (x_k + x_{k+1})/2$, where x_k is the beginning of the *k*th interval $x_k = x_{k-i} + \Delta x_k$, with $x_0 = 0$, so that the final formula for evaluating the Lauricella functions will be:

$$F_D(a;b_1,b_2,b_3,b_4;a+1;z_1,z_2,z_3,z_4) = \sum_{i=1}^{N} \frac{(x_i)^{a-1}}{(1-x_i z_1)^{b1}(1-x_i z_2)^{b2}(1-x_i z_3)^{b3}(1-x_i z_4)^{b4}} \Delta x_i \tag{14}$$

As no previous numerical calculations of the Lauricella functions were available for verifying the accuracy of our evaluations, we had to find recurrence relationships which can be used for this. So, we can prove:

$$\begin{aligned} &-\frac{z_1+z_2}{3-\tau} F_D(3-\tau;2-\nu,2-\nu,1+\nu,1+\nu;4-\tau;z_1,z_2,z_3,z_4) \\ &= -\frac{1}{2-\tau} F_D(2-\tau;1-\nu,1-\nu,1+\nu,1+\nu;3-\tau;z_1,z_2,z_3,z_4) \\ &-\frac{1}{2-\tau} F_D(2-\tau;2-\nu,2-\nu,1+\nu,1+\nu;3-\tau;z_1,z_2,z_3,z_4) \\ &-\frac{z_1 z_2}{4-\tau} F_D(4-\tau;2-\nu,2-\nu,1+\nu,1+\nu;5-\tau;z_1,z_2,z_3,z_4); \end{aligned} \tag{15}$$

$$\begin{aligned} &\frac{z_3+z_4}{3-\tau} F_D(3-\tau;1-\nu,1-\nu,2+\nu,2+\nu;4-\tau;z_1,z_2,z_3,z_4) \\ &= \frac{1}{2-\tau} F_D(2-\tau;1-\nu,1-\nu,2+\nu,2+\nu;3-\tau;z_1,z_2,z_3,z_4) \\ &-\frac{1}{2-\tau} F_D(2-\tau;1-\nu,1-\nu,1+\nu,1+\nu;3-\tau;z_1,z_2,z_3,z_4) \\ &+\frac{z_3 z_4}{4-\tau} F_D(4-\tau;2-\nu,2-\nu,2+\nu,2+\nu;5-\tau;z_1,z_2,z_3,z_4) \end{aligned} \tag{16}$$

and also, the following relationships:

$$\frac{1}{2-\tau}F_D(2-\tau;-\nu,-\nu,2+\nu,2+\nu;3-\tau;z_1,z_2,z_3,z_4)$$
$$=\frac{1}{2-\tau}F_D(2-\tau;1-\nu,1-\nu,2+\nu,2+\nu;3-\tau;z_1,z_2,z_3,z_4) \quad (17)$$
$$-\frac{z_1+z_2}{3-\tau}F_D(3-\tau;1-\nu,1-\nu,2+\nu,2+\nu;4-\tau;z_1,z_2,z_3,z_4)$$
$$+\frac{z_1z_2}{4-\tau}F_D(4-\tau;1-\nu,1-\nu,2+\nu,2+\nu;5-\tau;z_1,z_2,z_3,z_4)$$

A more general relationship, that has a nontranscendental term useful for comparison is:

$$b_3\left[\frac{1}{a}F_D(a;b_1,b_1,b_3+1,b_3+1;a+1;z_1,z_2,z_3,z_4)\right.$$
$$\left.-\frac{z_3z_4}{a+2}F_D(a+2;b_1,b_1,b_3+1,b_3+1;a+3;z_1,z_2,z_3,z_4)\right]$$
$$+b_1\left[\frac{1}{a}F_D(a;b_1+1,b_1+1,b_3,b_3;a+1;z_1,z_2,z_3,z_4)\right. \quad (18)$$
$$\left.-\frac{z_1z_2}{a+2}F_D(a+2;b_1+1,b_1+1,b_3,b_3;a+3;z_1,z_2,z_3,z_4)\right]$$
$$-\frac{b_1+b_3-a}{a}F_D(a;b_1,b_1,b_3,b_3;a+1;z_1,z_2,z_3,z_4)$$
$$=(1-z_1-z_2+z_1z_2)^{-b_1}(1-z_3-z_4+z_3z_4)^{-b_3}$$

We found, for the numerical parameters and variables provided by the physical context of the Compton scattering of X and gamma ray, that these recurrence relationships, implying several Lauricella functions are satisfied with errors in the range 10^{-6}-10^{-10} %, for a number of intervals, N, between 50-500. Further increasing of the number of sampling points was not necessary, as the required precision was usually obtained at 10^2-3.10^2 points.

Also, taking in (18) the parameters $b_1=1-\nu$, $b_3=1+\nu$ and $a=2-\tau$ we obtain the following relationships that finally reduce the number of Lauricella functions involved in the expressions of amplitudes, only *four* such functions being needed.

$$(1+\nu)\left[\frac{1}{2-\tau}F_D(2-\tau;1-\nu,1-\nu,2+\nu,2+\nu;3-\tau;z_1,z_2,z_3,z_4)\right.$$
$$\left.-\frac{z_3z_4}{4-\tau}F_D(4-\tau;1-\nu,1-\nu,2+\nu,2+\nu;5-\tau;z_1,z_2,z_3,z_4)\right] \quad (19)$$
$$=(\nu-1)\left[\frac{1}{2-\tau}F_D(2-\tau;2-\nu,2-\nu,1+\nu,1+\nu;3-\tau;z_1,z_2,z_3,z_4)\right.$$
$$\left.-\frac{z_1z_2}{4-\tau}F_D(4-\tau;2-\nu,2-\nu,1+\nu,1+\nu;5-\tau;z_1,z_2,z_3,z_4)\right]$$
$$+\frac{\tau}{2-\tau}F_D(2-\tau;1-\nu,1-\nu,1+\nu,1+\nu;3-\tau;z_1,z_2,z_3,z_4)$$
$$+(1-z_1-z_2+z_1z_2)^{-(1-\nu)}(1-z_3-z_4+z_3z_4)^{-(1+\nu)}$$

In Fig. 4 we present the comparison between our calculations for the doubly differential cross-section with the corresponding S-matrix calculations of Bergstrom *et al* [1]. It may be observed a very good concordance even for high values of the incident photon energies.

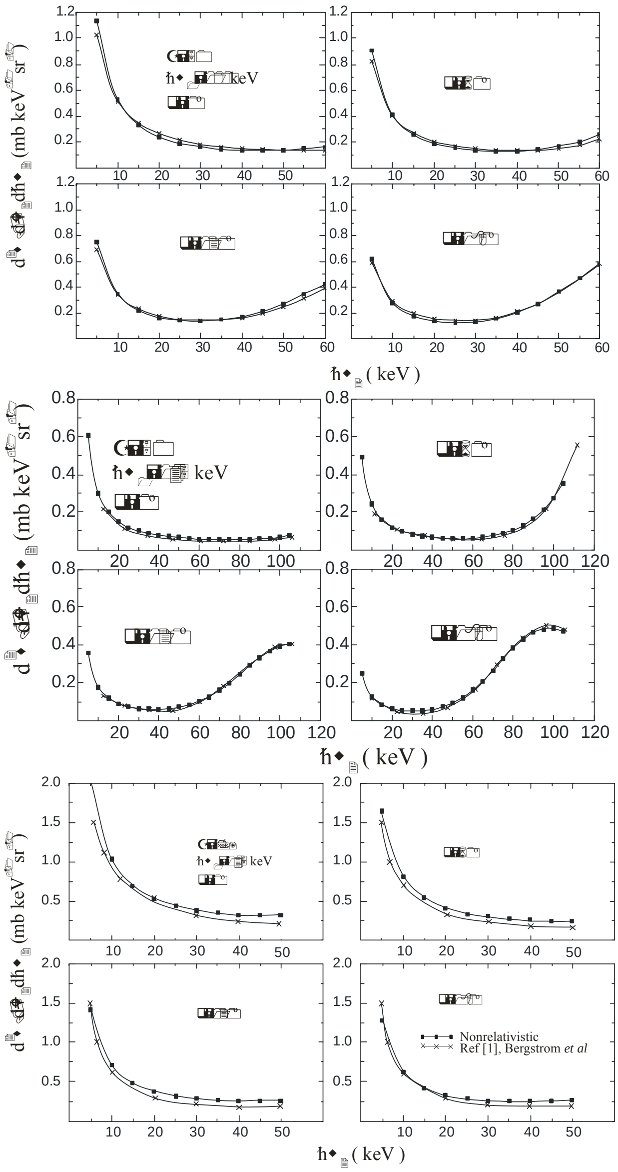

FIG. 4. Comparison of present results (boxes) with the corresponding S-matrix calculations (x) of Bergstrom et al [1].

The parameters of the physical process give a higher oscillating behavior of the Lauricella function integrand as the energies of the incident particle increase, so we tested the accuracy of our evaluations at some higher values, until 10 MeV, and we found that even for this domain the calculus of Lauricella functions is accurate. The same problem occurs for heavy elements, so it is important to observe the good concordance with the S-matrix results even for Z=79 (Fig. 5), and energies beyond the X-ray, well inside the gamma-ray domain.

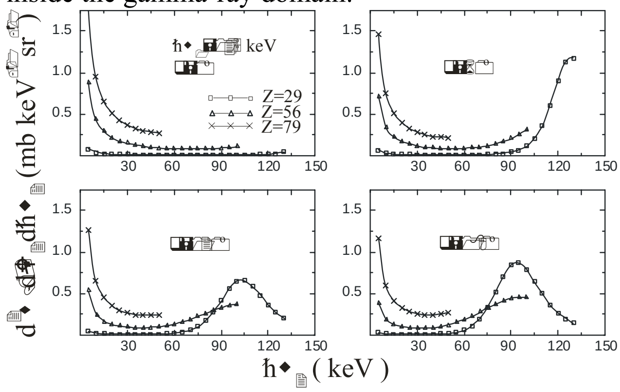

FIG. 5. Compton doubly differential cross-sections for intermediate and high Z values, at 145 keV. One may observe that when Z decreases, the Compton peak is higher and narrower.

All these come to prove that a better accuracy of the model and the calculus is achieved for smaller incident photon energies and lighter elements. Indeed, our curves and Bergstrom *et al* curves are practically superposed for the whole X-ray spectrum and any Z.

4. Conclusions

Starting from the analytical expression of the triply differential Compton cross-section [5], we perform the integration over the solid angles, implying the numerical evaluation of the Lauricella functions.

The economy obtained in the evaluation time, due to our efficient sampling method, allowed us to further integrate the products of the calculated Lauricella functions over the solid angle, as the calculus of the doubly differential cross section requires, and eventually a supplementary integration over the spectrum for obtaining the single differential cross section.

Our method takes into account the full form of Lauricella functions, with two of their variables depending on the direction of the final electron and photon, thus correctly considering the multipoles and retardation.

The good agreement with the results obtained through fundamentally different methods, shown in fig. 4, proves once more the validity and the applicability of our analytically formulae as well as the accuracy of our calculations. We consider that our work completely describes the X-ray Compton scattering by the K-shell bound electrons. Also, due to the accuracy of the evaluation of Lauricella functions at much higher energies, the calculus of the Compton cross-sections can be extended to hard gamma-ray domain.

As Hostler proved [8], the Green function for Dirac equation with coulombian field may be expressed iteratively as a sum of self adjoint operators applied to a coulombian Schrodinger equation Green function who's parameters are given by relativistic kinematics. This leads to similar Lauricella and Appell functions in the inelastic and elastic scattering amplitudes, respectively, but with changed parameters and variables, making possible to extend our numerical method to the relativistic calculus of the two photon atomic processes.

Acknowledgements

This work was partially supported by the Romanian National Council for University Scientific Research (CNCSIS) under Grant A 1576/2005.

References:

[1] P. M. Bergstrom, T. Surič, K. Pisk, R. H. Pratt, Phys Rev A 48, 1134 (1993).
[2] J. Schwinger, Journal of Mathematical Physics 5,1606 (1964).
[3] M.Gavrila, A.Costescu, Phys. Rev A 2, 1752 (1970).
[4] F. Schnaidt, Ann. Physik 21, 89 (1934).
[5] A. Costescu, S. Spanulescu, (to be published).
[6] William H. Press, Saul A. Teukolski, William T. Vetterling, Brian P. Flannery, Numerical Recipes in C, Cambridge University Press, 1992.
[7] Stephen Wolfram, The Mathematica Book, Wolfram Media, 2003.
[8] L. Hostler, Journal of Mathematical Physics 5, 591(1964).