Anomalous Rayleigh scattering of X-rays and photoeffect by inner shell electrons

A. Costescu(1), K. Karim(1), M. Moldovan(2), S. Spanulescu(3) and C.Stoica(1)

(1) Department of Physics, University of Bucharest
(2) Department of Physics, UMF Targu Mures
(3) Hyperion University of Bucharest

Rayleigh scattering by 1s electrons

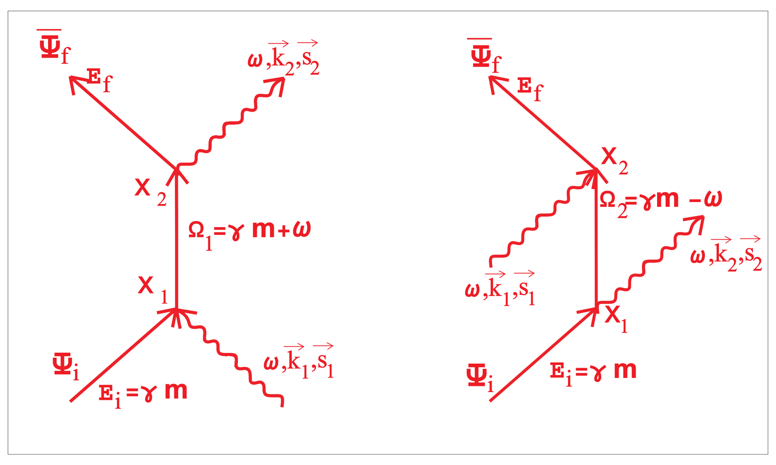

Figure 1. Feynman diagrams for elastic scattering of photons by 1s electrons

The invariant elastic scattering amplitudes in the case of 1s electrons

$M(\omega, \ ) = O(\ ) \quad P(\Omega_1, \ ) \quad P(\Omega_2, \ ) \qquad N(\omega, \ ) = \quad Q(\Omega_1, \ ) \quad Q(\Omega_2, \ )$

For energies above the 1s ionization threshold

$$P_{nr}(\Omega_1) = 2^3(\ Z)^8 \frac{m^4}{\omega^4} \frac{\omega}{\omega_{th}} \quad 1^{\frac{3}{2}} \frac{F_1(2 \ \ ^{nr}_1; 2,2;3 \ \ ^{nr}_1; x_1^{nr}, x_2^{nr})}{2 \ \ ^{nr}_1} ie^{4i \ ^{nr}_0}$$

$$Q_{nr}(\Omega_1) = \ 2^5(\ Z)^{10} \frac{m^4}{\omega^4} \frac{\omega}{\omega_{th}} \quad 1^{\frac{5}{2}} \frac{F_1(3 \ \ ^{nr}_1; 3,3;4 \ \ ^{nr}_1; x_1^{nr}, x_2^{nr})}{3 \ \ ^{nr}_1} ie^{6i \ ^{nr}_0}$$

$$^{nr}_1 = \begin{cases} 1 \ \dfrac{\omega}{\omega_{th}}^{\frac{1}{2}}, & pentru\ \omega < \omega_{th} \\ i \ \dfrac{\omega}{\omega_{th}} \ 1^{\frac{1}{2}}, & pentru\ \omega_{th} \ \ \omega \end{cases} \qquad ^{nr}_2 = 1 \ \dfrac{\omega}{\omega_{th}}^{\frac{1}{2}}$$

$$\omega_{th} = (1 \quad)m \qquad \omega_{pp} = (1 \quad)m = m \quad E_0$$

The Appell functions variables are given by the followig relationships

$$p = x_1^{nr} x_2^{nr} = \ ^2_{nr}(\Omega) \qquad s = x_1^{nr} \quad x_2^{nr} = 2 \ 1 \ \ 2 \ \ ^2Z^2 \ \ 1\text{m}\frac{\omega}{\omega_{th}} \ \sin^2 \frac{}{2} \quad _{nr}(\Omega)$$

$$_{nr}(\Omega_1) = e^{2i \ ^{nr}_0} \qquad _{nr}(\Omega_2) = \frac{1 \ \ \dfrac{\omega}{^2Z^2m} \quad 1 \ \ \dfrac{\omega}{\omega_{th}}^{\frac{1}{2}}}{1 \ \ \dfrac{\omega}{^2Z^2m} \quad 1 \ \ \dfrac{\omega}{\omega_{th}}^{\frac{1}{2}}}$$

$$^{nr}_0 = \begin{cases} \arctan \dfrac{\sqrt{\dfrac{\omega}{\omega_{th}} \ 1}}{1 \ \ \dfrac{E_0\omega}{^2Z^2m^2}}, & \text{dac a } \omega \ \dfrac{^2Z^2m^2}{E_0} \\ \arctan \dfrac{\sqrt{\dfrac{\omega}{\omega_{th}} \ 1}}{\dfrac{E_0\omega}{^2Z^2m^2} \ \ 1}, & \text{dac a } \omega > \dfrac{^2Z^2m^2}{E_0} \end{cases}$$

Table 1. Comparison of the total photoeffect cross section with the numerical results of Scofield [1] in the case of Z=79

ω(eV)	σ(barn)[1]	σ(barn)	ε%
40000	2557.4	2584.96	- 1.08
50000	1393.	1395.04	- 0.15
60000	839.79	839.64	0.02
80000	372.35	374.972	- 0.7
100000	196.33	200.134	- 1.94
150000	60.663	63.894	- 5.33
200000	26.376	28.509	- 8.09
300000	8.3403	9.237	- 10.75

For energies below the 1s ionization threshold the scattering amplitudes are:

$$P_{nr}(\Omega) = 2^3(\ Z)^8 \frac{m^4}{\omega_{th}^4} \ 1\text{m}\frac{\omega}{\omega_{th}}^{\frac{3}{2}} \frac{1}{D^2} \frac{F_1(2 \ \ ^{nr}; 2,2;3 \ \ ^{nr}; x_1^{nr}, x_2^{nr})}{2 \ \ ^{nr}}$$

$$Q_{nr}(\Omega) = 2^5(\ Z)^{10} \frac{m^4}{\omega_{th}^4} \frac{\omega^2}{\omega_{th}^2} \ 1\text{m}\frac{\omega}{\omega_{th}}^{\frac{5}{2}} \frac{1}{D^3} \frac{F_1(3 \ \ ^{nr}; 3,3;4 \ \ ^{nr}; x_1^{nr}, x_2^{nr})}{3 \ \ ^{nr}} \qquad D = \ 1 \ \frac{E_0}{m} \ 1 \ \sqrt{1\text{m}\frac{\omega}{\omega_{th}}} \ \text{m}\frac{E_0}{m}\frac{\omega}{\omega_{th}}^2 \ \ ^2Z^2 \frac{\omega}{\omega_{th}}$$

The total photoeffect cross section for the 1s electrons is:

$$\sigma_{1s}^{PH} = \frac{32}{3} \ ^2r_0^2E_0m^2 \ \ ^5Z^6 \frac{E_0 \quad \omega}{\omega^4} \frac{e^{\ | \ ^{nr}_1|} \quad ^{nr}(\omega)}{1 \ \ e^{2 \ | \ ^{nr}_1|}}$$

Table 2. Comparison of the total photoeffect cross section with the numerical results of Scofield [1] in the case of Z=26

ω	$\sigma_{1s}^{ph}(CSS07_22Sc)$	Z_{ef}	σ_{1s}^{ph}	err
keV	barn	-	barn	%
1	2	3	4	5
8	24769			
8.990	19383.400 †	25.60	1.8981e+4	2.1
10	13889	25.60	1.4247e+4	-2.6
15	4648.1	25.60	4.6710e+3	-0.5
20	2077.8	25.61	2.0749e+3	0.1
30	646.03	25.61	6.4633e+2	-0.0
40	276.35	25.62	2.7912e+2	-1.0
50	141.6	25.63	1.4480e+2	-2.3
60	81.565	25.64	8.4522e+1	-3.6
80	33.885	25.67	3.6102e+1	-6.5
100	17.064	25.70	1.8670e+1	-9.4
150	4.8937	25.77	5.6700	-15.9
200	2.0311	25.83	2.4518	-20.7

Table 3. Comparison of the total photoeffect cross section with the numerical results of Scofield [1] in the case of Z=22

ω	$\sigma_{1s}^{ph}(CSS07_22Sc)$	Z_{ef}	σ_{1s}^{ph}	err
keV	barn	-	barn	%
1	2	3	4	5
20.11	10607		1.0352e+4 å	-2.4
24.092	7854.27 †	41.59	6.9628e+3	12.8
30	3770.1	41.60	3.8308e+3	-1.6
40	1723.6	41.60	1.7314e+3	-0.5
50	925.19	41.60	9.2850e+2	-0.4
60	551.84	41.61	5.5610e+2	-0.8
80	241.04	41.62	2.4656e+2	-2.3
100	125.79	41.64	1.3095e+2	-4.1
150	38.213	41.68	4.1536e+1	-8.7
200	16.441	41.73	1.8490e+1	-12.5
300	5.1309	41.81	5.9865	-16.7

Rayleigh scattering by 2s electrons

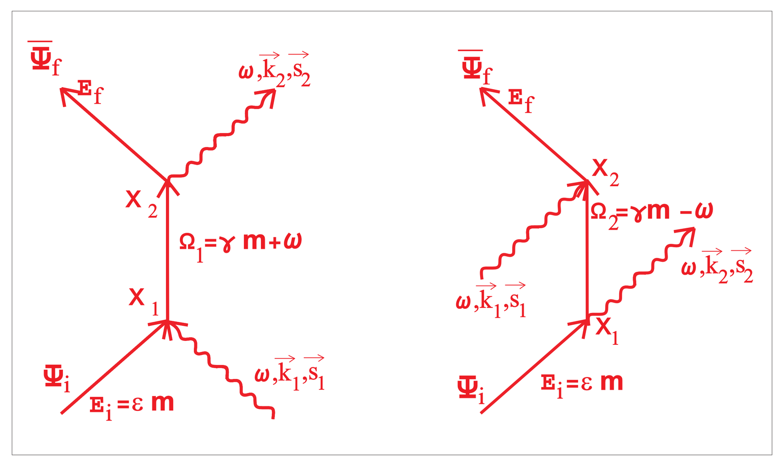

Figure 2. Feynman diagrams for elastic scattering of photons by 2s electrons

The invariant elastic scattering amplitudes in the case of 2s electrons

$$P_{NR}(\Omega, \ ) = \ 16 \ ^5 \ \frac{3}{2}(1 \quad)^4 m^4 \frac{\Omega^2}{\omega^2} \ ^4 \frac{X^7}{d^8} \frac{F_1(4 \quad ;4,4;5 \quad ;x_1,x_2)}{(4 \quad)}$$
$$\frac{X^5}{d^6} \frac{F_1(3 \quad ;3,3;4 \quad ;x_1,x_2)}{(3 \quad)}$$
$$(1 \quad)^2m^2 \ 1 \ \ 2\frac{m}{\omega} \ 1 \ \ \frac{3}{16} \ ^2Z^2\frac{m}{\omega} \quad ^2$$
$$\frac{X^3}{d^4} \frac{F_1(2 \quad ;2,2;3 \quad ;x_1,x_2)}{(2 \quad)}$$
$$1\text{m}\frac{1}{4} \ ^2Z^2(1 \quad)\frac{\Omega}{\omega}\text{m}\frac{1}{8} \ ^2Z^2(1 \quad)^2\frac{\Omega}{\omega} \quad \frac{^2Z^2}{2}(1 \quad)\frac{\omega_{th}^2}{\omega^2}$$
$$\frac{^2Z^2}{4}\frac{m}{\omega} \ 1 \ \ \frac{\omega_{th}}{m}^4 \ \frac{1}{1 \ \ \frac{^2}{4}^3}$$
$$1 \ \ \frac{1}{4}(1 \quad)^2\frac{\Omega}{\omega} \ \frac{1}{2} \quad 1 \ \ \frac{^2Z^2}{8}\frac{\Omega}{\omega} \quad ^2$$

$$Q_{NR}(\Omega, \ ) = 3 \ 2^{11} \ ^5\omega^2(1 \quad)^2m^4 \ ^2 \ 1 \quad \frac{1}{4\omega^2}(\ X^2 \ \ \frac{1}{2}(1 \quad)m^2) \ ^2$$
$$\frac{X^9}{d^{10}} \frac{F_1(5 \quad ;5,5;6 \quad ;x_1,x_2)}{(5 \quad)} \ 3 \ 2^8 \ ^5\omega^2(1 \quad)m^2$$
$$4 \ \ 3 \quad \frac{1}{4\omega^2} \ ^2 \quad X^2(7 \quad 2) \ \ 2\omega^2 \ \ \frac{5}{2}(1 \quad)m^2 \quad ^2Z^2\Omega^2$$
$$\frac{X^7}{d^8} \frac{F_1(4 \quad ;4,4;5 \quad ;x_1,x_2)}{(4 \quad)} \ 2^8 \ ^5\omega^2 \ 1 \ \ \frac{3}{8}(1 \quad) \quad \frac{5}{8} \ ^2Z^2\frac{X^2}{\omega^2}$$
$$\varepsilon \ \frac{3}{4}(1 \quad) \quad \frac{^2Z^2}{2} \ \frac{m}{\omega} \ \ \frac{1}{8} \ ^2Z^2(1 \quad)\frac{m^2}{\omega^2} \ \ \frac{3}{8} \ ^2Z^2(1 \quad)\frac{X^2}{\omega^2}$$
$$\frac{X^5}{d^6} \frac{F_1(3 \quad ;3,3;4 \quad ;x_1,x_2)}{(3 \quad)} \ \frac{3}{16} \ \frac{^2Z^2}{1 \ \ \frac{^2}{4}^4}(1 \quad)^2\varepsilon$$

The total photoeffect cross section for the 2s electrons is:

$$\sigma_{2s}^{PH} = \frac{4}{3} \ ^2 \ r_c^2(\ Z_{ef})^6 \frac{m^2}{\omega^2}\frac{\Omega_1}{\omega} \ \frac{E_{2s}\omega \quad \frac{3}{8} \ ^2Z_{ef}^2m^2}{\omega^2} \ \frac{e^{\ | \ _1|} \quad _1(\omega)}{1 \ \ e^{2 \ | \ _1|}} \ 1 \ \ \frac{2}{5}(1 \quad)^2\frac{m}{\omega}$$

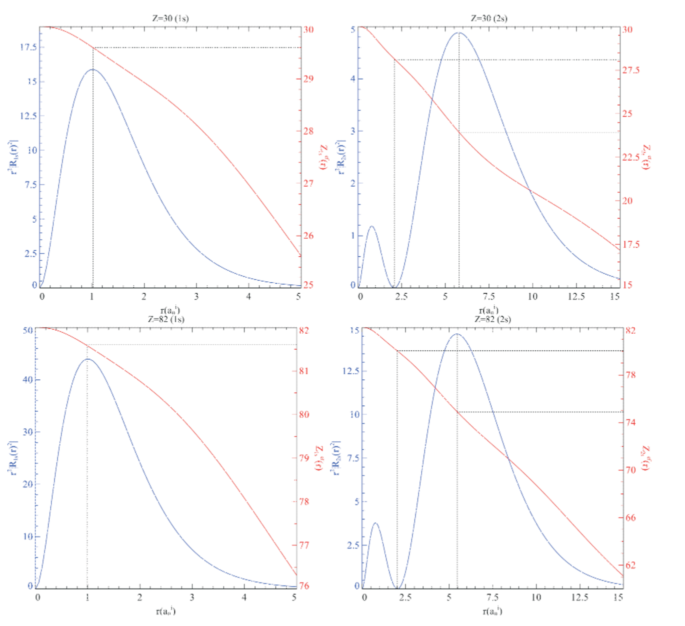

Figure 3: Effective charge and the Hartree-Fock probability density of the 1s electrons (left) and 2s electrons (right) in the case of neutral Zn atom (upper) and neutral Pb atom (lower)

Table 4. Rayleigh distribution and the ratio between the scattering amplitudes by 1s and 2s electrons and the numerical results of Kissell [2] for the whole atom, for Z=79

ϕ(deg)	σ(barn)	Im $A_\perp$ (%)	Re $A_\perp$ (%)	Im $A_\parallel$ (%)	Re $A_\parallel$ (%)
0	138.359	89.31	4.57	89.31	4.57
10	134.397	89.39	10.1	89.52	10.2
20	123.389	89.62	19.14	90.14	19.88
30	107.594	89.98	26.38	91.15	28.76
40	89.7972	90.42	33.38	92.57	39.
50	72.4809	90.9	42.87	94.49	55.08
60	57.3775	91.39	51.77	97.34	75.91
70	45.4183	91.83	57.32	-	-
80	36.8963	92.21	60.43	-	-
90	31.6727	92.49	62.8	-	-
100	29.3429	92.69	65.49	84.68	- 7.65
110	29.3509	92.79	68.62	88.37	32.75
120	31.0674	92.82	72.08	90.13	50.88
130	33.8473	92.79	75.57	91.14	62.57
140	37.0754	92.73	78.79	91.75	71.11
150	40.2032	92.65	81.56	92.13	77.39
160	42.7772	92.58	83.6	92.36	81.86
170	44.4601	92.53	85.	92.48	84.39
180	45.0444	92.52	85.37	92.52	85.37

Table 5. The invariant amplitudes for Rayleigh scattering of the photons on the 2s electrons for energies below the ionization threshold in the case of Z=79

ω(eV)	P(Ω_1)	P(Ω_2)	*O* - P(Ω_1)- P(Ω_2)
1000	0.523	0.48	- 0.0027
1500	0.536	0.47	- 0.0062
2000	0.55	0.461	- 0.0111
2500	0.565	0.453	- 0.0176
3000	0.581	0.445	- 0.0257
3500	0.598	0.437	- 0.0356
4000	0.617	0.43	- 0.0475
4500	0.638	0.423	- 0.0615
5000	0.661	0.417	- 0.078
5500	0.687	0.41	- 0.0974
6000	0.716	0.404	- 0.1201
6500	0.748	0.399	- 0.1467
7000	0.785	0.393	- 0.1782
7500	0.828	0.388	- 0.2156
8000	0.878	0.383	- 0.2606

Acknowledgement

The work of Cristian Stoica was supported by the strategic grant POSDRU/89/1.5/S/58852, Project "Postdoctoral programme for training scientific researchers" cofinanced by the European Social Found

1. Scofield J. H., Lawrence Radiation Laboratory Report No. CRL 51326, Livermore
2. Bergstrom P. M., Kissel L., Pratt R. H., Costescu A., Acta Crystallogr. A53 (1997)
3. Costescu A., Spanulescu S., Stoica C., J. Phys. B 40 (2007) 2995-3014
4. Costescu A.,Karim K., Moldovan M.,Spanulescu S., Stoica C., J. Phys. B 44 (2011) 045204