The total cross-sections for the photoeffect for 2S-subshell bound electrons and pair production with the created electron in the 2S subshell for photon energies above 1 MeV

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Considering the contributions of the main term of the relativistic Coulombian Green function given by Hostler [J. Math. Phys. 5, 591 (1964)] to the second order of the S-matrix element and taking into account only the large components of Dirac spinor of the 2S subshell, we have obtained the imaginary part of the Rayleigh amplitudes in terms of elementary functions. Thereby, simple and high accurate formulae for the total cross-sections for photoeffect and pair production with the electron created in the 2S subshell are obtained via the optical theorem. Comparing the predictions given by our formulae with the full relativistic numerical calculations of Kissel et al [Phys. Rev. A 22, 1970 (1980)] and Scofield [LLRL, Internal Report (1973)], a good agreement is found for low and intermediate Z values if screening effects are taken into account, for photon energies above the pair production threshold energy. We present our numerical results for the total photoeffect and pair production cross-sections for the 2S subshell of Zn and Ag atoms, for various photon energies.

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I. INTRODUCTION

The S matrix element for Rayleigh scattering by 2S bound electrons of an initial photon with momentum \( \mathbf{k}_1 = \omega \mathbf{\hat{v}}_1 \) and polarization vector \( \mathbf{\hat{s}}_1 \) and a final photon with momentum \( \mathbf{k}_2 = \omega \mathbf{\hat{v}}_2 \) and polarization vector \( \mathbf{\hat{s}}_2 \) is:

\[
\mathcal{M} = M(\omega, \theta)(\mathbf{\hat{s}}_1 \mathbf{\hat{s}}_2) + N(\omega, \theta)(\mathbf{\hat{s}}_1 \mathbf{\hat{v}}_2)(\mathbf{\hat{s}}_2 \mathbf{\hat{v}}_1) \tag{1.1}
\]

where \( \theta \) is the photon scattering angle, and the invariant amplitudes \( M \) and \( N \) are:

\[
M(\omega, \theta) = O - P(\Omega_1, \theta) - P(\Omega_2, \theta) \tag{1.2}
\]

\[
N(\omega, \theta) = Q(\Omega_1, \theta) + Q(\Omega_2, \theta)
\]

In the following we give the expression of the amplitude \( P(\Omega, \theta) \) which is the only term which has an imaginary in the case of forward scattering:

\[
P(\Omega, \theta) = \frac{\omega + \omega_{pp}}{2m} \left\{ \varepsilon^5 \frac{\lambda^2}{8m^2 \omega^2} \left[ \frac{\alpha Z \eta \Omega - 4 (\eta^2 + \varepsilon m \omega)}{(1 + \frac{\Delta^2}{4})^2} + \frac{2 (\eta^2 + \varepsilon m \omega) + \frac{\Delta^2}{4}}{(1 + \frac{\Delta^2}{4})^3} \right] + 16 \frac{\lambda^2}{X^2} \left[ \varepsilon^2 + \left( 1 + \frac{\tau^2}{4} \right) \frac{\alpha^2 Z^2 \Omega^2}{2 \omega^2} - \frac{\alpha^2 Z^2 \varepsilon \Omega}{2 \omega^2} (\eta^2 + \varepsilon m \omega) \right] \frac{X}{d^3(\Omega)} F_1(2 - \tau, 2, 2, 3 - \tau; x_1, x_2) \frac{X}{d^6(\Omega)} F_1(3 - \tau, 3, 3, 4 - \tau; x_1, x_2) \right\} \tag{1.3}
\]

with the parameters:

\[
\Omega_1 = \gamma m + \omega, \Omega_2 = \gamma m - \omega = -|\Omega_2|, \tag{1.4}
\]

\[
\gamma = (1 - \alpha^2 Z^2)^{1/2}, \lambda = \alpha Z m, \omega_{pp} = (1 + \gamma) m,
\]

\[
\eta = \frac{\lambda}{2\varepsilon}, \varepsilon = \sqrt{\frac{1 + \gamma}{2}}, \tau = \frac{\alpha Z \Omega}{X}, \Delta = k_1 - k_2
\]

\[
X^2 = -\omega^2 + 2 \varepsilon m \omega + \eta^2 \text{ with } \text{Re}[X] > 0 \tag{1.5}
\]

The function \( O \) is the atomic form factor, while \( F_1(a; b_1, b_2; c; x_1, x_2) \) is the Appell hypergeometric function of four parameters and two complex variables given by the relationships:
\[ x_1 x_2 = p(\Omega) = \left[ \frac{d^* (\Omega)}{d (\Omega)} \right]^2 = \xi^2 \]  

(1.6)

\[ x_1 + x_2 = s (\Omega) = 2\xi - \frac{16X^2\omega^2 \sin^2 \theta}{d^2 (\Omega)} \]

(1.7)

with

\[ d (\Omega) = 2 (\eta_1^2 \mp \varepsilon m\omega + \eta X) \]  

(1.8)

\[ d^* (\Omega) = 2 (\eta_1^2 \mp \varepsilon m\omega - \eta X) \]  

(1.9)

In the equations (1.3-1.6) the upper sign corresponds to the case \( \Omega = \Omega_1 \), while the lower sign corresponds to the case \( \Omega = \Omega_2 \).

We want to point out that the first term in the equation (1.3) which has no transcendental function and always real expression comes from recurrence relationships among Appell's functions, having no connection with the atomic factor.

Actually, using one more recurrence relationship, the equation (1.3) may be expressed in terms of only two independent Appell’s functions.

According to the optical theorem, the imaginary part of the Rayleigh amplitude for forward scattering allows to get the total photoeffect and pair production cross-sections:

\[ \sigma_{ph} = \frac{4\pi m}{\alpha \omega} r_0^2 \left| \text{Im} [P(\Omega_1, 0)] \right| \]  

(1.10)

\[ \sigma_{pp} = \frac{4\pi m}{\alpha \omega} r_0^2 \left| \text{Im} [P(\Omega_2, 0)] \right| \]  

(1.11)

II. THE TOTAL CROSS-SECTION OF THE PHOTOELECTRIC EFFECT AND PAIR PRODUCTION IN THE CASE OF 2s SUBSHELL

Taking into account only the main term of the relativistic Coulombian Green function given by Hostler and considering only the large components of the 2s subshell Dirac spinor, we obtain the imaginary part of the amplitude for the forward elastic scattering of photons by 2s subshell electrons as follows:

\[
\left| \text{Im} [P(\Omega_1, 0)] \right| = 2\frac{\omega + \omega_{pp}}{2m} \frac{\lambda X_1^2 \left( 1 + |\tau_1|^2 \right)}{6m^4 \omega^4} \frac{\pi |\tau_1| |X_1|}{e^{-|\tau_1|\chi_1}} \frac{e^{-|\tau_1|\chi_1}}{e^{\pi|\tau_1|\chi_1}} \left. \right| \left[ e^2 + \frac{\lambda^2 X_1^2}{2m^2 \omega^2} - \frac{\varepsilon \alpha^2 Z^2 \Omega_1}{2m\omega^2} (\eta^2 - \varepsilon m\omega) \right] \left. \right| \\
\left| \text{Im} [P(\Omega_2, 0)] \right| = 2\frac{\omega - \omega_{pp}}{2m} \frac{\lambda X_2^2 \left( 1 + |\tau_2|^2 \right)}{6m^4 \omega^4} \frac{\pi |\tau_2| |X_2|}{e^{-|\tau_2|\chi_2}} \frac{e^{-|\tau_2|\chi_2}}{e^{\pi|\tau_2|\chi_2}} \left. \right| \left[ e^2 + \frac{\lambda^2 X_2^2}{2m^2 \omega^2} + \frac{\varepsilon \alpha^2 Z^2 \Omega_2}{2m\omega^2} (\eta^2 + \varepsilon m\omega) \right] \left. \right|
\]

where \( \lambda = \alpha Z m, \eta = \frac{\lambda}{2\varepsilon}, \omega_{pp} = (1 + \varepsilon)m, X_j = m^2 - \Omega_j^2 \) with \( \text{Re}[X_j] > 0, \tau_j = \frac{\alpha Z \Omega_j}{X_j^2}, j = 1, 2 \)

and

\[ \chi_1 = \pi - 2 \arctan \frac{\eta |X_1|}{\varepsilon m\omega - \eta^2}, \chi_2 = \pi - 2 \arctan \frac{\eta |X_2|}{\varepsilon m\omega + \eta^2}, \text{for } \omega > \omega_{pp} \]

(2.3)

Observing that \( |\tau_j|^2 |X_j|^2 = \alpha^2 Z^2 \Omega_j^2 \) and \( 1 - \frac{\varepsilon^2}{\eta^2} = \varepsilon^2 \) and using eqs. (1.10) - (2.2) we get the 2S subshell photoeffect and pair production total cross-sections:

\[
\sigma_{ph} = 2\frac{\pi^2}{3} \frac{\alpha^2 Z^6 \omega + \omega_{pp}}{\omega^2} \left( \frac{|X_1|^2 + \alpha^2 Z^2 \Omega_1^2}{4} \right) \frac{\varepsilon |\tau_1| \chi_1}{\varepsilon m\omega - \eta^2} \left[ e^2 - \frac{\lambda^2 |X_1|^2}{2m^2 \omega^2} - \frac{\varepsilon \alpha^2 Z^2 \Omega_1}{2m\omega^2} (\eta^2 - \varepsilon m\omega) \right] \left. \right| \left. \right|
\]

(2.4)

\[
\sigma_{pp} = 2\frac{\pi^2}{3} \frac{\alpha^2 Z^6 \omega - \omega_{pp}}{\omega^2} \left( \frac{|X_2|^2 + \alpha^2 Z^2 \Omega_2^2}{4} \right) \frac{\varepsilon |\tau_2| \chi_2}{\varepsilon m\omega + \eta^2} \left[ e^2 - \frac{\lambda^2 |X_2|^2}{2m^2 \omega^2} + \frac{\varepsilon \alpha^2 Z^2 \Omega_2}{2m\omega^2} (\eta^2 + \varepsilon m\omega) \right] \left. \right| \left. \right|
\]

(2.5)
TABLE I: Photoeffect and pair production cross sections for Zn 2S subshell ($Z_{\text{eff}}=28$).

| Energy (keV) | Pair production cross section (mb) | Photoeffect cross section (mb) | Cross sections ratio |
|-------------|-----------------------------------|--------------------------------|----------------------|
| 1022        | $1.647 \times 10^{-10}$           | 5.95752                        | 3.61 $\times 10^{10}$ |
| 1100        | 0.000695                          | 5.07405                        | 7298.68              |
| 1200        | 0.00554                           | 4.21312                        | 759.343              |
| 1500        | 0.036731                          | 2.66716                        | 72.61                |
| 2000        | 0.085664                          | 1.54132                        | 17.9925              |
| 2754        | 0.119357                          | 0.881717                       | 7.38719              |
| 3000        | 0.123683                          | 0.765855                       | 6.19209              |
| 3500        | 0.12716                           | 0.599167                       | 4.7119               |
| 4000        | 0.126442                          | 0.488387                       | 3.86253              |
| 4807        | 0.121266                          | 0.372844                       | 3.0746               |
| 5000        | 0.119682                          | 0.352461                       | 2.9447               |
| 5500        | 0.115336                          | 0.308281                       | 2.67289              |
| 6000        | 0.110871                          | 0.273507                       | 2.4669               |
| 6500        | 0.106464                          | 0.245495                       | 2.3059               |
| 7000        | 0.102209                          | 0.222493                       | 2.17684              |
| 7500        | 0.0981532                         | 0.205295                       | 2.0712               |

Obviously, in the above formulae, the screening effects must be considered because in a 2S state they are important. In a roughly screening model which allows keeping the coulombian shape of the spinors a realistic approach is to consider an effective charge $Z_{\text{eff}} = Z - 2$ which has to be used in all numerical calculations.

III. NUMERICAL RESULTS AND CONCLUSIONS

Using our analytical formulae for the cross sections for 2S subshell electrons we get the numerical numerical results in Table I, Table II, figure 1 and figure 2.

One may notice that changing the atomic number with it’s effective value keeps the shape of the graphics, decreasing the whole spectrum values. Also, it may be seen that the pair production cross section has a slight maximum, followed by a slow decreasing region.

Comparing the predictions given by our formulae with the full relativistic numerical calculations of Kissel et al and Scofield, a good agreement within 10% is found for low and intermediate Z values if screening effects are taken into account, for photon energies above the pair production threshold up to 5 MeV.

TABLE II: Photoeffect and pair production cross sections for Ag 2S subshell ($Z_{\text{eff}}=45$).

| Energy (keV) | Pair production cross section (mb) | Photoeffect cross section (mb) | Cross sections ratio |
|-------------|-----------------------------------|--------------------------------|----------------------|
| 1022        | $2.10404 \times 10^{-8}$          | 43.9758                        | 2.09 $\times 10^{7}$  |
| 1100        | 0.0035494                         | 37.5046                        | 10566.4              |
| 1200        | 0.0329387                         | 31.1846                        | 946.746              |
| 1500        | 0.242849                          | 19.7968                        | 81.519               |
| 2000        | 0.586374                          | 11.4659                        | 19.554               |
| 2754        | 0.826457                          | 6.56745                        | 17.9451              |
| 3000        | 0.857616                          | 5.70553                        | 6.65278              |
| 3500        | 0.883206                          | 4.46472                        | 5.05513              |
| 4000        | 0.878962                          | 3.63959                        | 4.14078              |
| 4807        | 0.8435                            | 2.77862                        | 3.29416              |
| 5000        | 0.83255                           | 2.62671                        | 3.15501              |
| 5500        | 0.80242                           | 2.2974                         | 2.86309              |
| 6000        | 0.77130                           | 2.03818                        | 2.64218              |
| 6500        | 0.740752                          | 1.82936                        | 2.4696               |
| 7000        | 0.711145                          | 1.65788                        | 2.33128              |
| 7500        | 0.682912                          | 1.51476                        | 2.21809              |
FIG. 1: Photoeffect (upper) and pair production (lower) cross sections for 2S-subshell of Ag calculated for Z=47 (red) respectively effective atomic number Z$_{\text{eff}}$=45 (green).

FIG. 2: Photoeffect (red) and pair production (green) cross sections for Ag 2S subshell (Z$_{\text{eff}}$=45).

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