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# Perturbative calculation of the cross section in double ionization by high-energy Compton scattering

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**Abstract.** In this paper we investigate double ionization in high-energy Compton scattering from the He-atom including both the shake-off mechanism and a perturbative correction to that mechanism. The correction is calculated in second-order perturbation theory and includes Coulomb electron-electron interaction in addition to the correlation in the ground state of the He-atom. Our calculations for the ratio of double to single cross section cover the range from 30 to 300 keV of impact photon energy and explain the slow convergence of the ratio towards the asymptotic value.

**PACS.** 32.80.Fb Photoionization of atoms and ions – 32.80.Cy Atomic scattering, cross sections, and form factors; Compton scattering

## 1 Introduction

Double ionization of two-electron atoms serves as a tool for the investigation of the electron-electron correlation [1]. In particular, high-energy double ionization of the He-atom via Compton scattering is dominated by the shake-off ($SO$) mechanism, as a result of an averaged correlation between two electrons at all positions in the initial atom state. Final state correlations are neglected in the $SO$ mechanism on the basis of the sudden approximation assumption. As a consequence, the ratio of double to single cross section $R_C$ approaches a constant (asymptotic) value at sufficiently high impact energy. This was demonstrated by the asymptotic formula for $R_C$ in the impulse approximation calculations for Compton scattering ionization and the value $R_C = 0.797\%$ was obtained for the He-atom with the Hylleraas-type wave function [2]. The '$A^2$' calculations of Andersson and Burgdörfer [3], for the He-atom with a highly correlated initial state wave function and an approximately correlated or uncorrelated final state wave function, predicted a decreasing toward the same constant value $R_C \approx 0.8\%$. Many–body perturbation theory (MBPT) calculations of Hino et al. [4], although performed at much lower energies, are consistent with these findings [5].

A calculation which includes the electron – electron interaction in the final and initial states was performed by Mikhaĭlov and Mikhaĭlov [6]. However, they presented only the asymptotic ratio of double to single cross section (value $R_C = 1.2\%$) for the He-atom at high-energy impact.

Experimental findings of Spielberger et al. [7] and Becker et al. [8] on He-atom double ionization in the energy range 40–120 keV exhibit a rather slow convergence towards the asymptotic value of $R_C$. These results indicate the persistent influence of final-state correlations even at very high photon energies.

The calculations of Spielberger et al. [7] with $3C$ Coulombic wave functions in the final state reproduce this slow convergence toward the constant $R_C$. However, the $3C$ function contains the Coulomb electron-electron correlation in an approximate form and there is no a priori justification for its use, although this function is found valid in the asymptotic region of the configuration space.

In this paper we investigate double ionization in high-energy Compton scattering by developing a different approach which circumvents the above cited problems with the $3C$ function. We develop a perturbative approach which includes both the $SO$ mechanism and a perturbative correction to that mechanism. The correction is calculated in the second-order perturbation theory and includes the Coulomb electron-electron interaction besides the correlation in the ground state of the He-atom.

## 2 Approach to the process

Our considerations are based on the sudden approximation for Compton scattering and an additional interaction between ionized electrons during the process. By assuming only the sudden approximation we obtain the $SO$ amplitude, $A_{SO}$, which enables us to calculate rather constant

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ratio of double to single cross section at high energies. By allowing the electron – electron Coulomb interaction during the process of Compton scattering, we introduce an additional mechanism for double ionization. Accordingly, the ejection of the second electron is a consequence of the (Compton) electron – (bound) electron interaction, and it is described by the Coulomb correction amplitude $A_C$.

Our calculations are nonrelativistic and Compton scattering is calculated using the '$A^2$' term of the electron–photon interaction. For the ground state of the He-atom we use the effective charge variational wave function with $Z^* = 27/16$, which is symmetric in configuration space, because the two-electron spin function is spin singlet. Within the $A^2$ approximation [which cannot change the spin state] the final state is also spin singlet. The electron – electron interaction in the initial state is highly simplified within the model which we use. A better description can be incorporated by using convenient independent particle approximation orbitals through approaches such as the multiconfiguration Hartree-Fock or the configuration interaction approach [9]. In such a description one would also include $p$-states and higher angular momenta, in addition to the $s$-states which we use. However, the function which we use, with effective charge, already takes 90% of the effect, as discussed in [10]. When applied to the asymptotic formula [2], the variational wave function gives for the ratio of cross sections $R_C = 0.712\%$, which is somewhat below the true value $R_C = 0.797\%$.

For the wave function of the fast Compton electron we use a plane wave, because high energies and small $Z$ of the $He^+$ ion are involved. For the wave function of the second (slow) ejected electron we use the Coulombic wave for the $Z = 2$ field. For the electron intermediate states we use plane waves, and only the ground state of the $He^+$-ion since in single ionization of the He-atom the ground state of the $He^+$-ion participates in more than 90% of all events [2].

## 3 Formalism

According to the preceding discussion for the ground state of the He-atom, we use the variational wave function

$$\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \phi_0(1)\phi_0(2) = N_0^2\, \mathrm{e}^{-\eta_0(r_1+r_2)}, \tag{1}$$

where $r_{1,2}$ are radial coordinates of bound electrons, and $N_0$, $\eta_0$ are values of the parameters for the effective charge $Z^* = 27/16$.

Compton scattering is calculated by the standard $A^2$-term of the electron – photon interaction

$$H_{ep}(1) = 2\pi r_0 \frac{\boldsymbol{\epsilon}_1 \cdot \boldsymbol{\epsilon}_2}{\sqrt{\omega_1\omega_2}}\, \mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{r}_1}, \tag{2a}$$

where

$$\boldsymbol{k} = \boldsymbol{k}_1 - \boldsymbol{k}_2, \tag{2b}$$

and $\boldsymbol{r}_1$ is a coordinate of the fast Compton ejected electron. In equation (2), $\boldsymbol{\epsilon}_{1,2}$, $\omega_{1,2}$, $\boldsymbol{k}_{1,2}$ are polarizations, energies, and momenta of incident (index 1) and scattered (index 2) photons respectively, and $r_0$ is the classical electron radius. We employ $\hbar = c = 1$ units.

### 3.1 Shake-off mechanism

The amplitude, $A_{SO}$, for the $SO$ mechanism reads

$$A_{SO} = 2\pi r_0 \frac{\boldsymbol{\epsilon}_1 \cdot \boldsymbol{\epsilon}_2}{\sqrt{\omega_1\omega_2}}\, \left\langle \boldsymbol{p}_1 \left| \mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{r}} \right| \phi_0(1) \right\rangle \left\langle \boldsymbol{p}_2 \middle| \phi_0(2) \right\rangle, \tag{3}$$

where $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ are momenta of the fast and the slow electron, respectively.

In the high-energy limit the amplitude $A_{SO}$, given by equation (3), gives a simpler version of the more general formula for the ratio of double to total cross section derived in the impulse approximation calculation if the factorized wave function of the ground state is assumed [2].

### 3.2 Coulomb-interaction correction

The Coulomb-interaction correction to the $SO$ mechanism is represented by the amplitude $A_C$, which is calculated in the second-order perturbation theory, under the assumption of the preceding section, and which reads

$$A_C = \frac{1}{(2\pi)^3} \int \mathrm{d}\boldsymbol{p} \frac{M_1(\boldsymbol{p}) \cdot M_2(\boldsymbol{p})}{E - p^2/2m + \mathrm{i}\,\varepsilon}, \tag{4a}$$

with

$$\begin{aligned} M_1(\boldsymbol{p}) &= \left\langle \boldsymbol{p}_1 \boldsymbol{p}_2 \left| H_C(1,2) \right| \mathrm{e}^{\mathrm{i}\,\boldsymbol{p}\cdot\boldsymbol{r}_1}\, \phi_0^i(2) \right\rangle \\ M_2(\boldsymbol{p}) &= \left\langle \phi_0^i(2)\, \mathrm{e}^{-\mathrm{i}\,\boldsymbol{p}\cdot\boldsymbol{r}_1} \left| H_{ep}(1) \right| \phi_0(1)\phi_0(2) \right\rangle \end{aligned} \tag{4b}$$

and

$$E = \omega_1 - \omega_2 - I_0 + I_0^i, \tag{4c}$$

where $m$ is the mass of the electron, $I_0$ and $I_0^i$ represent the ground state energies of the He-atom and the $He^+$-ion respectively. In equation (4a) $\phi_0^i$ represents the ground state wave function of the $He^+$-ion, and $H_C$ represents the electron-electron Coulomb interaction of ionized electrons

$$H_C(1,2) = \frac{\alpha}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}, \tag{5}$$

where $\alpha = e^2/4\pi$ is the fine structure constant. The other symbols in equations (4), (5) are the same as in the preceding expressions.

For the evaluation of the amplitude $A_C$, equation (4a), we use the Coulombic wave function for the ground state of the $He^+$-ion as

$$\phi_0^i(2) = N_i\, \mathrm{e}^{\eta_i r_2}, \tag{6}$$

where $N_i$ and $\eta_i$ are Coulombic values of the parameters for $Z = 2$, and, according to our approach, we also use a plane wave for the fast ejected electron. A simple calculation leads to the amplitude $A_C$, given by equation (4a),

$$A_C = \frac{1}{(2\pi)^3} \int \mathrm{d}\boldsymbol{p} \frac{B_1(\boldsymbol{p}) B_2(\boldsymbol{p})}{E - p^2/2m + \mathrm{i}\,\varepsilon}. \tag{7}$$

In equation (7), the $B_1$ function is given by

$$B_1(\boldsymbol{p}) = 4\pi^2 r_0 \frac{\boldsymbol{\epsilon}_1 \cdot \boldsymbol{\epsilon}_2}{\sqrt{\omega_1\omega_2}} \eta_0 N_0 \frac{\left\langle \phi_0^i(2) \middle| \phi_0(2) \right\rangle}{\left[(\boldsymbol{p} - \boldsymbol{k})^2 + \eta_0^2\right]^2}. \tag{8}$$

The function $B_2$ is given by

$$B_2(\boldsymbol{p}) = \frac{4\pi}{(\boldsymbol{p}-\boldsymbol{p}_1)^2} I(\boldsymbol{p}), \tag{9a}$$

where $I(\boldsymbol{p})$ is an integral of the form

$$I(\boldsymbol{p}) = \int \mathrm{d}\boldsymbol{r}\, \mathrm{e}^{-\mathrm{i}(\boldsymbol{p}-\boldsymbol{p}_1)\cdot\boldsymbol{r}}\, \phi^*_{\boldsymbol{p}_2}(\boldsymbol{r})\phi^i_0(\boldsymbol{r}). \tag{9b}$$

In equation (9b), $\phi_{\boldsymbol{p}_2}$ represents a wave function of the slow ejected electron for momentum $\boldsymbol{p}_2$. In the calculations we have used a Coulombic wave for $Z = 2$.

### 3.3 Double-ionization cross section

The amplitude $A_C$ given by equation (4a) or equation (7) is a perturbative correction to the $SO$ amplitude $A_{SO}$ given by equation (3), when high energies are considered. The cross section for double ionization is defined by coherent superposition of these amplitudes and it reads

$$\mathrm{d}\sigma^{++} = \frac{1}{(2\pi)^8} \sum_{\mathrm{pol}} |A_{SO} + A_C|^2 \times \delta(\omega_1 - \omega_2 - I_0 - \varepsilon_1 - \varepsilon_2)\, \mathrm{d}\boldsymbol{k}_2\, \mathrm{d}\boldsymbol{p}_1\, \mathrm{d}\boldsymbol{p}_2. \tag{10}$$

For the sake of discussion, we also introduce $\mathrm{d}\sigma^{++}_{SO}$ and $\mathrm{d}\sigma^{++}_{C}$ by using in equation (10) only $A_{SO}$ or $A_C$ amplitude respectively. In equation (10) $\varepsilon_{1,2}$ represent fast and slow electron energy respectively and $\Sigma_{\mathrm{pol}}$ stands for the sum over photon polarizations.

To prepare the amplitude $A_C$ given by equation (4) for numerical evaluation and calculation of the corresponding cross section, we separate the $p$-integration in two parts: a $\delta$-part and a principal value (PV) part, according to the well-known relation

$$\frac{1}{E - p^2/2m + \mathrm{i}\,\varepsilon} = -\,\mathrm{i}\,\pi\delta(E - p^2/2m) + PV\frac{1}{E - p^2/2m}. \tag{11}$$

However, our numerical analysis shows that for high-energies, when the first electron is fast and the second is slow, the $PV$-part is orders of magnitude smaller than the $\delta$-part and therefore we have neglected it.

## 4 Results and discussion

Our Coulomb correction has been calculated by assuming a plane wave as a wave function of the Compton ejected fast electron. We have investigated the accuracy of employment of plane waves in the calculation of singly differential cross sections (with respect to the scattered photon angle $\mathrm{d}\Omega$) for double ionization based on the $SO$ mechanism. We compared the plane wave results with the results obtained by Coulombic function and we concluded that our plane wave calculations are accurate for incident photon energies above 30 keV.

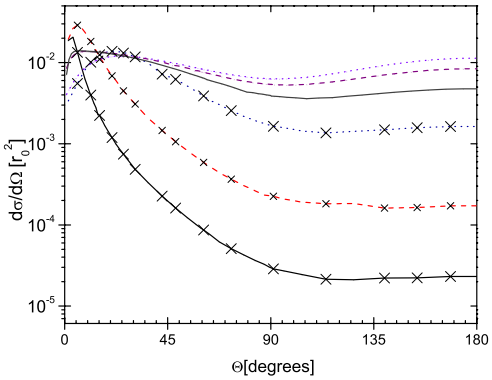


**Fig. 1.** Differential cross sections $\mathrm{d}\sigma^{++}_{SO}$ (lines without crosses) and $\mathrm{d}\sigma^{++}_{C}$ (lines with crosses $\times$) as functions of the scattered photon angle. Results for incident photon energies of 30 keV (dotted lines), 80 keV (dashes) and 200 keV (solid) are shown.

**Table 1.** Total cross sections for double ionization from the $SO$ mechanism and from the $C$-correction calculation.

| $\omega_1$[keV] | $\sigma^{++}_{SO}[r_0^2]$ | $\sigma^{++}_{C}[r_0^2]$ |
|---|---|---|
| 30 | $1.03 \times 10^{-1}$ | $4.36 \times 10^{-2}$ |
| 80 | $9.17 \times 10^{-2}$ | $1.42 \times 10^{-2}$ |
| 200 | $7.12 \times 10^{-2}$ | $2.90 \times 10^{-3}$ |

In Figure 1 we plot the singly differential cross sections $\mathrm{d}\sigma^{++}_{C}$ and $\mathrm{d}\sigma^{++}_{SO}$ as functions of the scattered photon angle at incident energies of 30, 80, and 200 keV. The lines with crosses ($\times$) show $\mathrm{d}\sigma^{++}_{C}$ while the lines without crosses show $\mathrm{d}\sigma^{++}_{SO}$. The respective integrated cross sections are shown in Table 1.

From these calculations one can observe two important features of the Coulomb interaction correction:

(a) at a given impact energy the importance of the correction increases at smaller scattering angles, being of the same order as the $SO$ value in the forward photon peak, and
(b) the contribution of the correction to the total cross section decreases with impact energy much faster than the contribution of the $SO$ mechanism.

From the values of the calculated cross sections we can mark the beginning of the asymptotic domain which is around 100 keV, where the Coulomb correction contributes less than 10% to the total cross section. At the energy of 150 keV this contribution is 5.5%.

In Figure 2 we show the ratio of double to single cross section $\sigma^{++}/\sigma^{+}$ as a function of impact photon energy. The cross section $\sigma^{+}$ is calculated by standard $A^2$ procedure. In the same graph we plot the values of the double to single ratio $\sigma^{++}_{SO}/\sigma^{+}$, where the double ionization cross sections are calculated for the $SO$ mechanism only. We also plot experimental values of the ratio for high energies, the same theoretical asymptotic estimates, and $3C$ calculations of [7]. One can observe that the ratio $R_{SO}$ increases with energy and approaches rather fast the asymptotic value $R_{SO} = 0.712\%$ (at the energy of 50 keV $R_{SO}$ is 0.7).

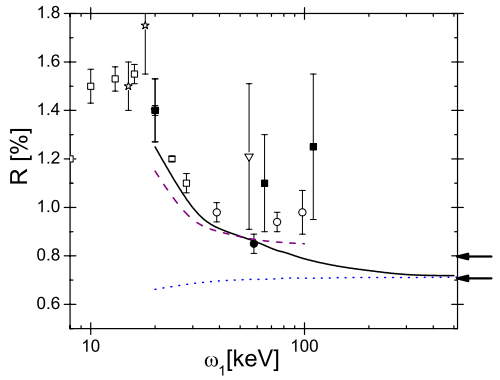


**Fig. 2.** Ratio of the double to single ionization cross section of helium as a function of incoming photon energy. The solid curve is obtained by using equation (10), while the dotted curve is obtained by the *SO* mechanism only. Experimental results: Spielberger et al. [7] (open circles), [11] (solid circles), Krässig et al. [12] (open squares), Wehlitz et al. [13] (triangle), Becker et al. [8] (solid squares), Levin et al. [14] (stars). The dashed line is the calculation with the 3*C* function [7]. The calculated values of $R_C^\infty$ [2], were obtained with initial state Hylleraas-type wave function (upper arrow) and variational wave function with $Z_{eff}$ (lower arrow).

From Figure 2 we may conclude that our perturbative approach to double ionization explains the energy dependence of the double to single ratio for high incident photon energy. Our calculations clearly demonstrate that the slow convergence of the ratio can be expressed within the first-order correction to the shake-off result. For the energy of 200 keV the Coulombic correction is only 4% of the *SO* cross section (see Tab. 1).

Our analysis shows that the slow convergence of the double to single ratio is a consequence of two factors:

i. there is a significant contribution of events with the low-energy transfer in Compton scattering even at high energies, i.e., the slow energy electrons for which *SO* is not valid;
ii. Coulomb interaction between ionized electrons is significant in the case of low-energy electron ejection.

The agreement of our calculations for the ratio with the existing experimental data is reasonably satisfactory, considering the approximations we have used.

## 5 Conclusions

In this work we have investigated the ionization of the He-atom in high-energy Compton scattering. We have developed an approach for double ionization which includes the shake-off mechanism as well as a perturbative correction influenced by the Coulomb interaction between ionized electrons. Our calculations for the ratio of double to single cross section cover the range from 30 to 300 keV of impact photon energy and explain the slow convergence of the ratio towards the asymptotic value. We have found that the ratio approaches the constant value within 10% at about 100 keV. The ratio of double to single ionization has been compared with experimental data and with the existing theoretical results. Our results agree reasonably well with the existing experimental data and the agreement is better with the data which display smaller error bars. Our results also confirm the results for the total cross section obtained by using the 3*C* functions. However, for more differential cross sections we expect a difference between our perturbative approach and the 3*C* approach.

We expect that this work will inspire further investigations, theoretical as well as experimental, of the high-energy Compton scattering ionization processes.

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